

## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	6078980	"alzheimer's" "beta-secretase activity" inhibition mammal prevent? control? reduc?	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	ON	2007/06/20 17:15
L2	35	"alzheimer's" "beta-secretase activity" inhibition mammal prevent? control? reduc?	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	AND	ON	2007/06/20 17:15

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NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 3 MAR 16 CASREACT coverage extended  
NEWS 4 MAR 20 MARPAT now updated daily  
NEWS 5 MAR 22 LWPI reloaded  
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 10 APR 30 CA/CAPLUS enhanced with 1870-1889 U.S. patent records  
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/CAPLUS Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/CAPLUS enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/CAPLUS enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 18 CA/CAPLUS to be enhanced with pre-1967 CAS Registry Numbers  
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.  
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FILE 'HOME' ENTERED AT 17:42:12 ON 20 JUN 2007

=> file registry

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1  
DICTIONARY FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1

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=>

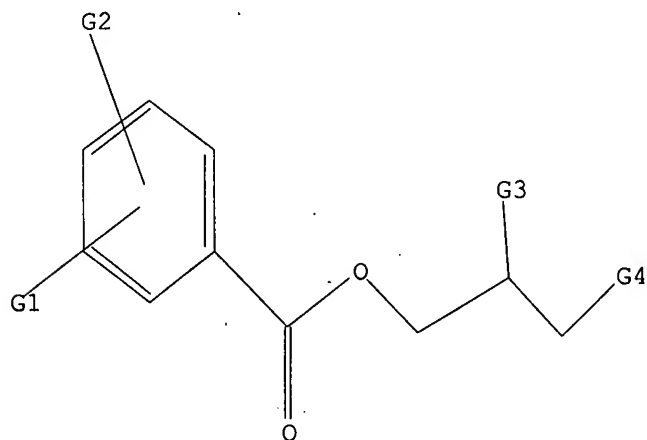
Uploading C:\Documents and Settings\jcho2\My Documents\10562470-1.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,O

G2 N,Ph

G3 O,N

G4 Ph,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 17:43:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 45746 TO ITERATE

100.0% PROCESSED 45746 ITERATIONS  
SEARCH TIME: 00.00.01

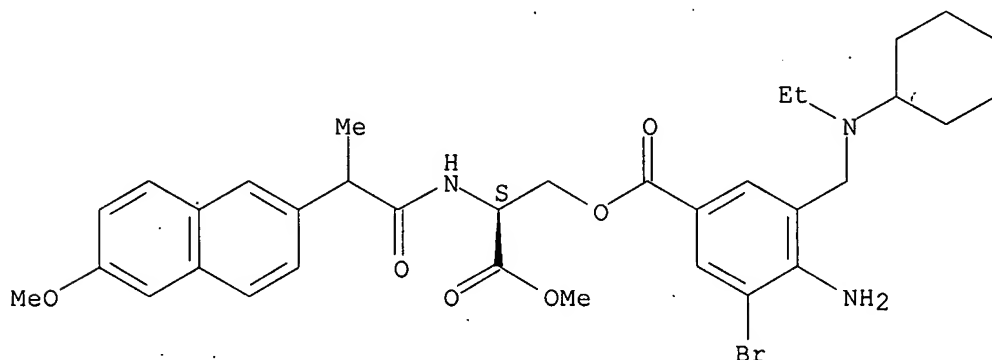
88 ANSWERS

L2 88 SEA SSS FUL L1

=> d scan

L2 88 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN L-Serine, N-[2-(6-methoxy-2-naphthalenyl)-1-oxopropyl]-, methyl ester,  
4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI)  
MF C34 H42 Br N3 O6

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):file caplus  
'FILE CAPLUS' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".  
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.55

172.76

FILE 'CAPLUS' ENTERED AT 17:43:46 ON 20 JUN 2007  
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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26  
FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

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<http://www.cas.org/infopolicy.html>

=> s 12

L3 30 L2

=> d 13 1-30 bib abs hitstr

L3 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:1191598 CAPLUS

DN 146:116781

TI Discovery of Oxadiazoyl Tertiary Carbinamine Inhibitors of  
 $\beta$ -Secretase (BACE-1)

AU Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel; Vacca, Joseph P.

CS Departments of Medicinal Chemistry, Structural Biology, Molecular Systems and Alzheimer's Research, Merck Research Laboratories, West Point, PA, 19486, USA

SO Journal of Medicinal Chemistry (2006), 49(25), 7270-7273

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

OS CASREACT 146:116781

AB We describe the discovery and optimization of tertiary carbinamine derived inhibitors of the enzyme  $\beta$ -secretase (BACE-1). These novel non-transition-state-derived ligands incorporate a single primary amine to interact with the catalytic aspartates of the target enzyme. Optimization of this series provided inhibitors with intrinsic and functional potency comparable to evolved transition state isostere derived inhibitors of BACE-1.

IT 918344-77-1 918344-77-1D, complexes with  
 $\beta$ -secretase

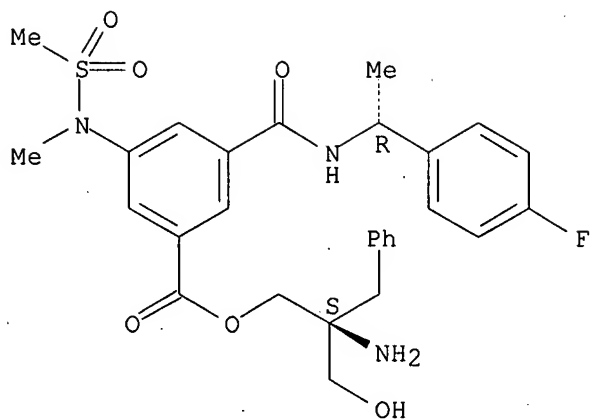
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL  
(Biological study)

(discovery of oxadiazoyl tertiary carbinamine inhibitors of  
 $\beta$ -secretase)

RN 918344-77-1 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

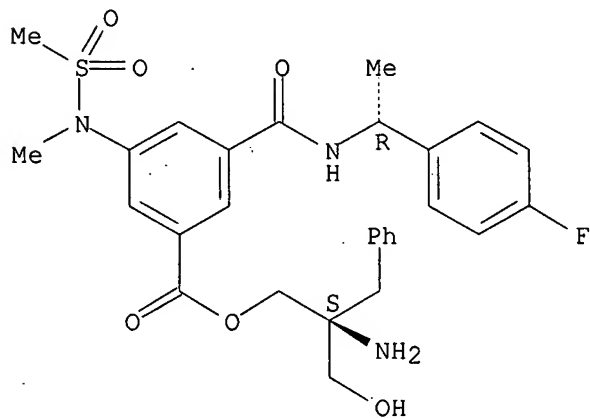
Absolute stereochemistry.



RN 918344-77-1 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:125835 CAPLUS

DN 144:202124

TI Phenylanthraquinones, and their electrophotographic photoconductors showing good durability and solvent resistance

IN Ichiguchi, Tetsuya

PA Kyocera Mita Industrial Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 47 pp.

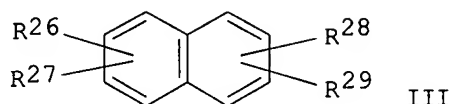
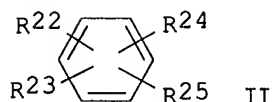
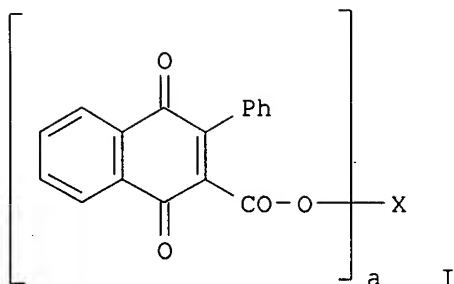
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2006036677	A	20060209	JP 2004-217855	20040726
PRAI	JP 2004-217855		20040726		
OS	MARPAT 144:202124				
GI					



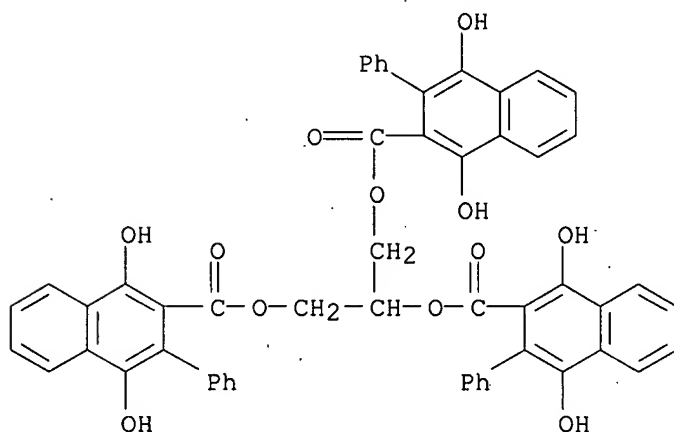
AB The naphthoquinones are I (X = trivalent group chosen from C<sub>6</sub>H<sub>3</sub>R<sub>1</sub>R<sub>2</sub>R<sub>3</sub>, R<sub>4</sub>CHR<sub>5</sub>R<sub>6</sub>, etc. when a = 3, tetravalent group chosen from tetravalent benzene II, tetravalent naphthalene III when a = 4; R<sub>1</sub>-R<sub>3</sub>, R<sub>22</sub>-R<sub>29</sub> = single bond, C<sub>1</sub>-8 alkylene, C<sub>2</sub>-8 alkylidene, etc.; R<sub>4</sub>-R<sub>6</sub> = single bond, C<sub>1</sub>-4 alkylene). The electrophotog. photoconductors contain charge generating agents, I as electron transporting agents, and binder resins. Thus, I (X = 1,3,5-benzenetrimethylene, a = 3) was manufactured and used for an electrophotog. photoconductor.

IT 875078-03-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(phenylnaphthoquinones as electron transporting materials for electrophotog. photoconductors showing good durability and solvent resistance)

RN 875078-03-8 CAPLUS

CN 2-Naphthalenecarboxylic acid, 1,4-dihydroxy-3-phenyl-, 1,2,3-propanetriyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

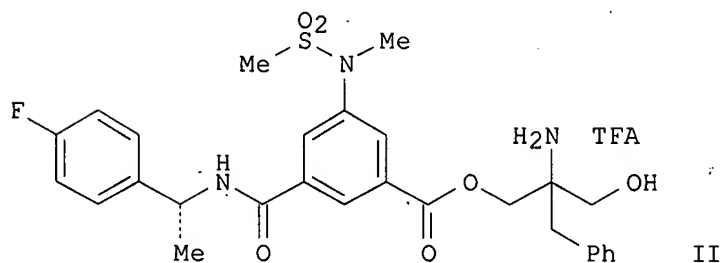
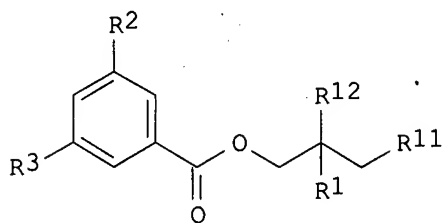
AN 2005:55021 CAPLUS

DN 142:134323

TI Preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease.

IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004255191	A1	20050120	AU 2004-255191	20040625
	CA 2530006	A1	20050120	CA 2004-2530006	20040625
	EP 1643986	A2	20060412	EP 2004-756168	20040625
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1909897	A	20070207	CN 2004-80018651	20040625
	US 2006149092	A1	20060706	US 2005-562470	20051222
PRAI	US 2003-484150P	P	20030701		
	WO 2004-US20525	W	20040625		
OS	MARPAT 142:134323				
GI					



AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as  $\beta$ -secretase inhibitors for



the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

IT 827039-49-6P 827039-50-9P 827039-51-0P  
827039-52-1P 827039-53-2P 827039-54-3P  
827039-55-4P 827039-56-5P 827039-60-1P  
827039-61-2P 827039-65-6P

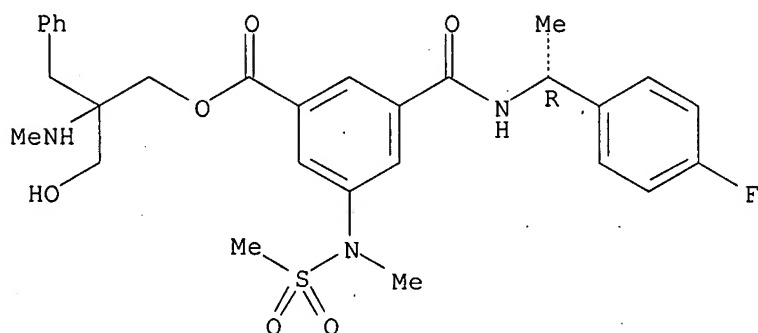
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-49-6 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

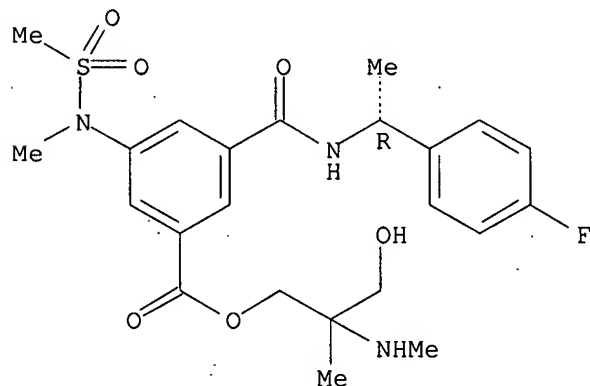
Absolute stereochemistry.



RN 827039-50-9 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-methyl-2-(methylamino)propyl ester (9CI) (CA INDEX NAME)

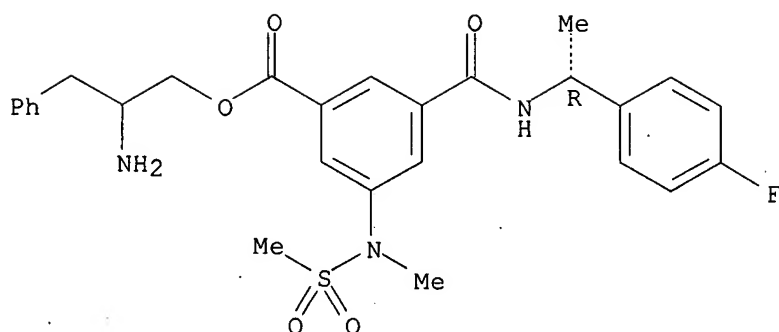
Absolute stereochemistry.



RN 827039-51-0 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-phenylpropyl ester (9CI) (CA INDEX NAME)

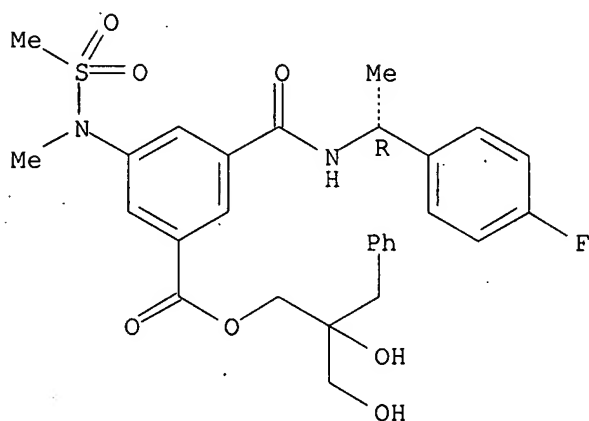
Absolute stereochemistry.



RN 827039-52-1 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2,3-dihydroxy-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

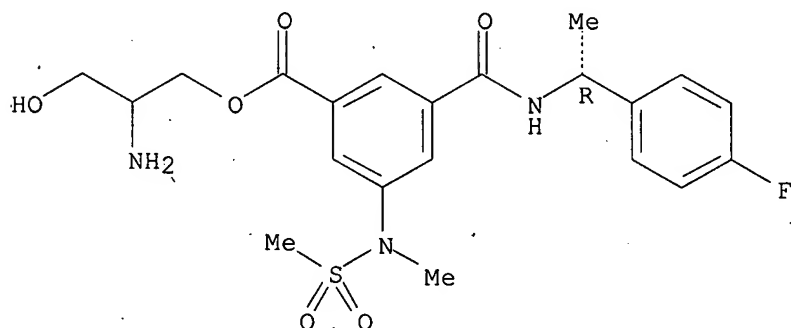
Absolute stereochemistry.



RN 827039-53-2 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI) (CA INDEX NAME)

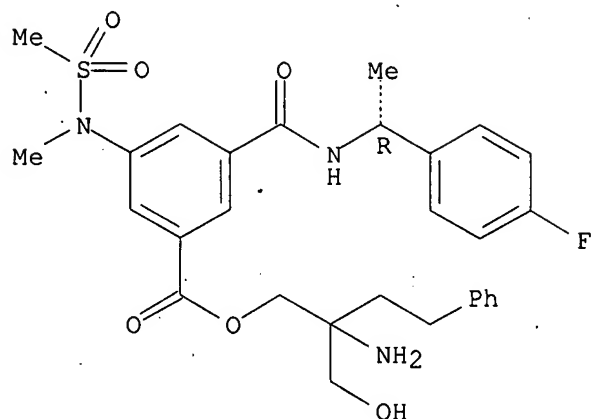
Absolute stereochemistry.



RN 827039-54-3 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-4-phenylbutyl ester (9CI) (CA INDEX NAME)

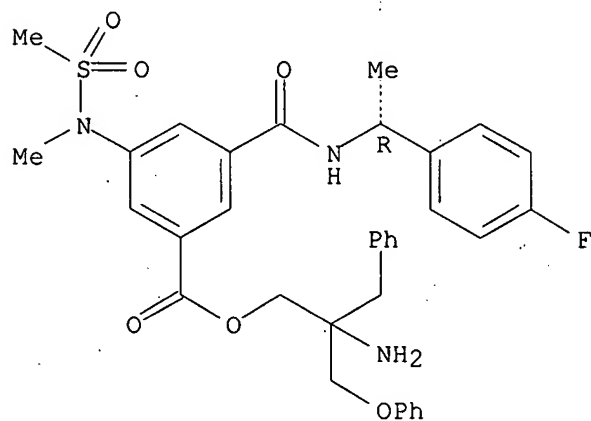
Absolute stereochemistry.



RN 827039-55-4 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(phenoxy)methyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)

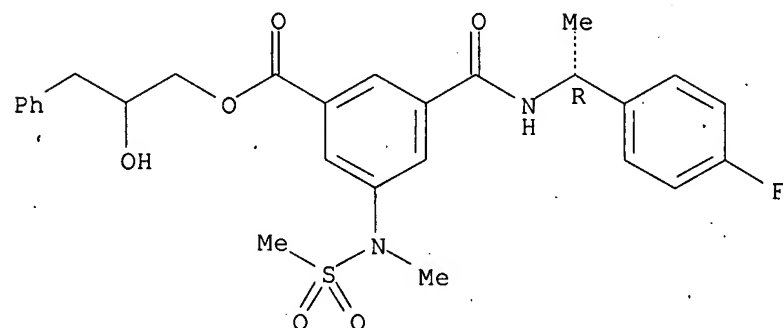
Absolute stereochemistry.



RN 827039-56-5 CAPLUS

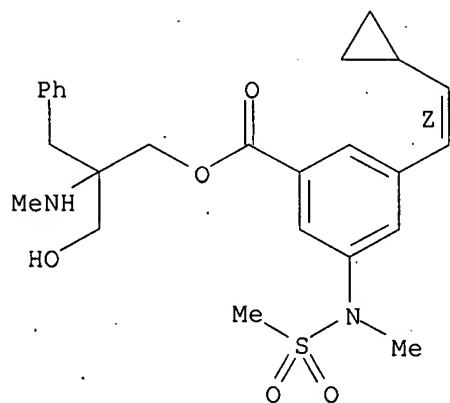
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-hydroxy-3-phenylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



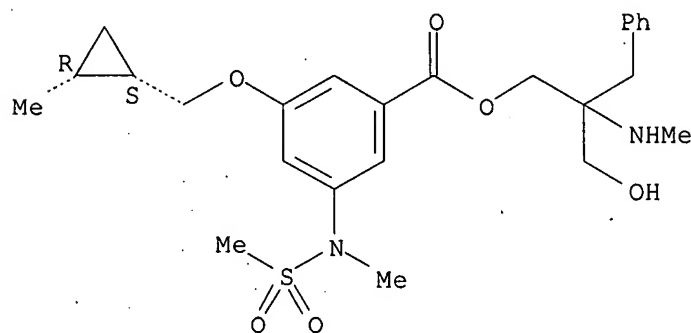
RN 827039-60-1 CAPLUS  
 CN Benzoic acid, 3-[(1Z)-2-cyclopropylethenyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



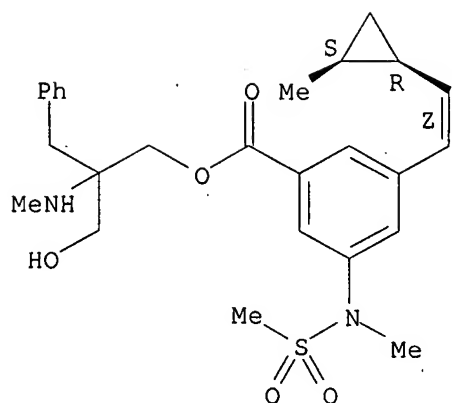
RN 827039-61-2 CAPLUS  
 CN Benzoic acid, 3-[[ (1R,2S)-2-methylcyclopropyl]methoxy]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 827039-65-6 CAPLUS  
 CN Benzoic acid, 3-[(1Z)-2-[(1R,2S)-2-methylcyclopropyl]ethenyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



IT 827039-74-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-74-7 CAPLUS

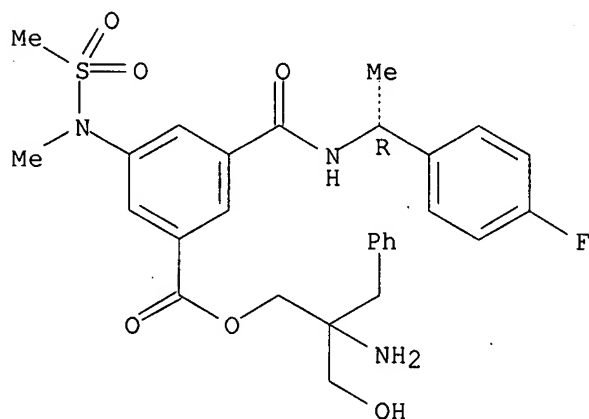
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 827039-73-6

CMF C28 H32 F N3 O6 S

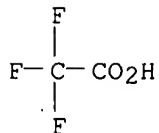
Absolute stereochemistry.



CM 2

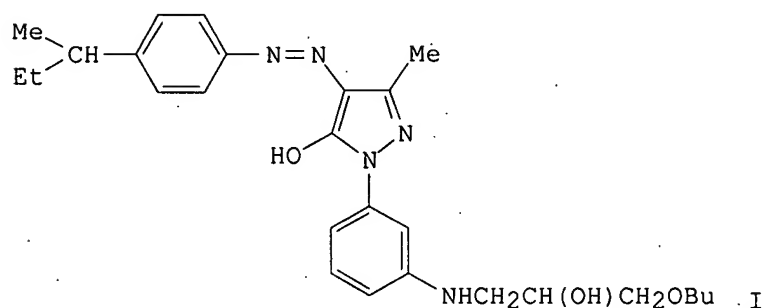
CRN 76-05-1

CMF C2 H F3 O2



L3 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1994:220382 CAPLUS  
 DN 120:220382  
 TI Liquid azo dyes and dye compositions and ink compositions using the same  
 IN Ono, Takashi; Yagyu, Tatsuya; Akase, Tetsumi  
 PA Orient Chemical Ind, Japan  
 SO Jpn. Kokai Tokkyo Koho, 15 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

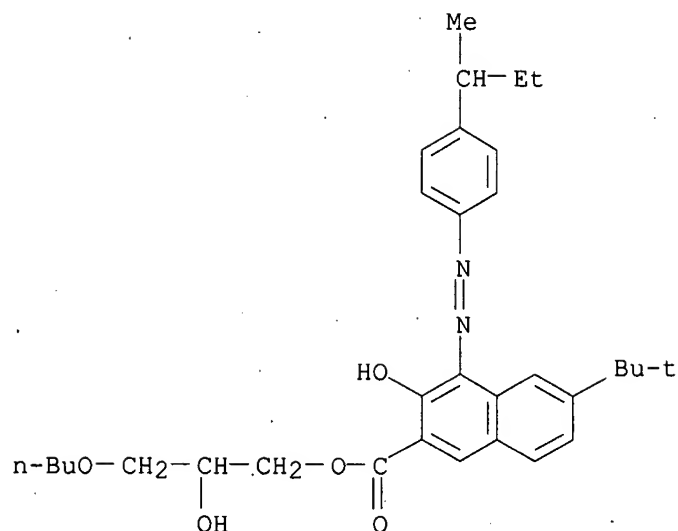
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05311084	A	19931122	JP 1992-121882	19920514
	JP 2986609	B2	19991206		
	US 5326866	A	19940705	US 1993-59666	19930512
	EP 573809	A1	19931215	EP 1993-107875	19930514
	EP 573809	B1	19980819		
	R: CH, DE, FR, GB, LI				
PRAI	JP 1992-121882	A	19920514		
OS	MARPAT 120:220382				
GI					



AB The title dyes soluble in alcs. and glycols are EtMeCHC6H4N:N(AN:N)nCpXCH2CH(OH)CH2OR [A = (un)substituted phenylene; n = 0, 1; Cp = pyrazolone derivative residue, naphthol derivative residue; X = NH, CO2; R = C3-12 alkyl].  
 1-(3-Aminophenyl)-3-methyl-5-pyrazolone was treated with Bu glycidyl ether in diethanolamine at 80-85° for 8 h, and the product coupled with diazotized p-sec-butylaniline to obtain yellow I. A marking ink providing wet- and lightfast markings comprised I 7, EtOH 68, benzyl alc. 5, Et lactate 10, and phenolic resin 10 parts.

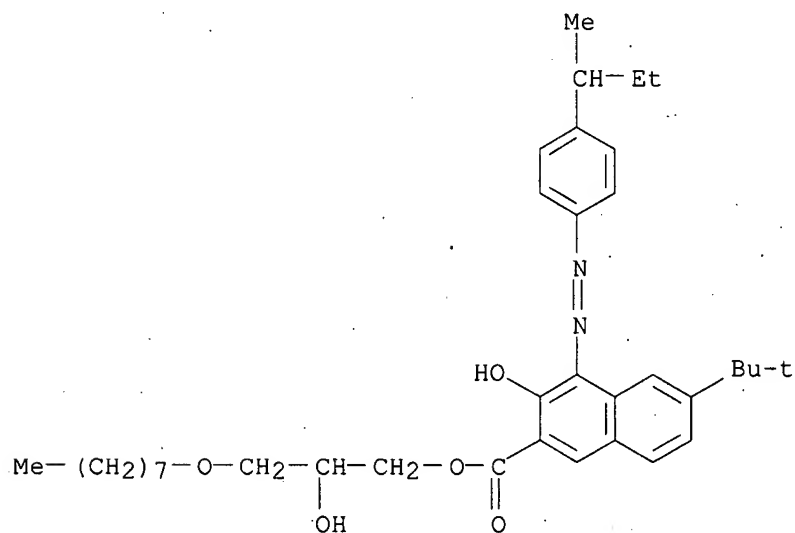
IT 154057-52-0P 154057-53-1P  
 RL: PREP (Preparation)  
 (manufacture of, dye, liquid, for inks)

RN 154057-52-0 CAPLUS  
 CN 2-Naphthalenecarboxylic acid, 6-(1,1-dimethylethyl)-3-hydroxy-4-[[4-(1-methylpropyl)phenyl]azo]-, 3-butoxy-2-hydroxypropyl ester (9CI) (CA INDEX NAME)



RN 154057-53-1 CAPLUS

CN 2-Naphthalenecarboxylic acid, 6-(1,1-dimethylethyl)-3-hydroxy-4-[[4-(1-methylpropyl)phenyl]azo]-, 2-hydroxy-3-(octyloxy)propyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1993:219790 CAPLUS

DN 118:219790

TI Thermal expansion of glassy polymers

AU Davy, K. W. M.; Braden, M.

CS Dent. Sch., Univ. London, London, E1 2AD, UK

SO Biomaterials (1992), 13(14), 1043-6

CODEN: BIMADU; ISSN: 0142-9612

DT Journal

LA English

AB The thermal expansion of a number of glassy polymers of interest in dentistry was studied using a quartz dilatometer. In some cases, the expansion was linear and therefore the coefficient of thermal expansion readily determined

Other

polymers exhibited non-linear behavior and values appropriate to different

temperature ranges are quoted. The linear coefficient of thermal expansion was, to a first approximation, a function of both the molar volume and van der Waal's volume

of the repeating unit.

IT 147187-18-6

RL: PROC (Process)

(thermal expansion of, for dental materials)

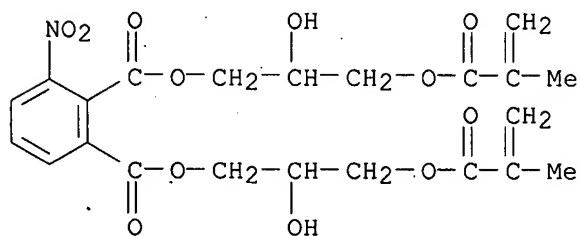
RN 147187-18-6 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3-nitro-, bis[2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl] ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 147187-17-5

CMF C22 H25 N O12



L3 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1992:37119 CAPLUS

DN 116:37119

TI Hydroxyalkyl amino-substituted triiodobenzoates and addition polymers of triiodo compounds for x-ray contrast materials for the gastrointestinal tract

IN Sovak, Milos

PA USA

SO Can. Pat. Appl., 36 pp.

CODEN: CPXXEB

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2031739	A1	19910609	CA 1990-2031739	19901207
	NO 9005299	A	19910610	NO 1990-5299	19901207
	EP 436316	A1	19910710	EP 1990-313363	19901207
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AU 9067910	A	19910613	AU 1990-67910	19901210
	AU 637435	B2	19930527		
	JP 04208232	A	19920729	JP 1990-415693	19901210
PRAI	US 1989-448073	A	19891208		
	US 1990-574300	A	19900828		

OS MARPAT 116:37119

AB Hydroxyalkyl amino-substituted triiodobenzoates, wherein the remaining position is substituted with amino or carboxy, are provided. These compds. have low solubility in the gastrointestinal tract, but are resorbable from extravisceral body cavities and are useful as contrast media for the plain radiog. of the GI tract. Also, addition polymers comprising triiodo compds. bonded through an amino N to a nonoxocarbonyl group of an addition polymerizable monomer are provided. These polymers are water-soluble, physiol. acceptable agents useful for computer tomog. of the GI tract. A radiopaque water-soluble copolymer with low I content was prepared from acrylamide, 5-N-acrylamido-2,4,6-triiodoisophthalic acid, and



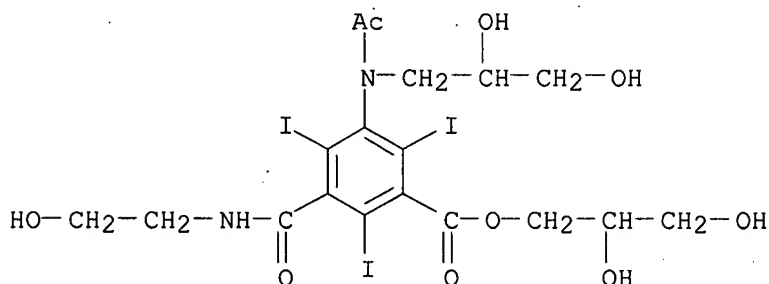
N,N'-methylene-bis-acrylamide. The copolymer in water was treated with charcoal at 70-75° to remove monomers, filtered, diluted with an EDTA-containing solution, autoclaved. The copolymer coated the gastrointestinal wall, was uniformly dispersed, gave no imaging artifacts, and delineated the entire tract with the same intensity of contrast throughout. The material also did not precipitate but seeped along the intestinal wall even in the presence of intestinal contents.

IT 138308-44-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as x-ray contrast agent for gastrointestinal tract imaging)

RN 138308-44-8 CAPLUS

CN Benzoic acid, 3-[acetyl(2,3-dihydroxypropyl)amino]-5-[[2-hydroxyethyl)amino]carbonyl]-2,4,6-triiodo-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

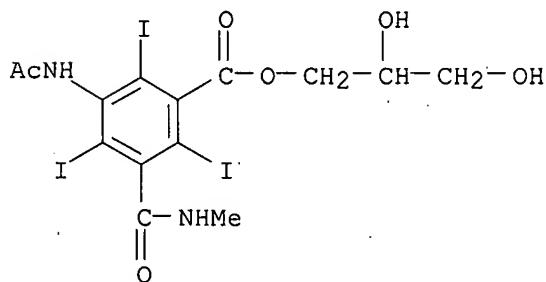


IT 138308-48-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, x-ray contrast agent for gastrointestinal tract imaging)

RN 138308-48-2 CAPLUS

CN Benzoic acid, 3-(acetyl(2,3-dihydroxypropyl)amino)-5-[[2-hydroxyethyl)amino]carbonyl]-2,4,6-triiodo-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:607264 CAPLUS

DN 115:207264

TI Synthesis and characterization of 1-methacryl-3-salicyloyl-2-hydroxypropane and its derivatives - a structure-reactivity kinetic study

AU Babu, N. Vijaya; Rajanna, K. C.; Rao, C. Janaki Ram

CS Nizam Coll., Osmania Univ., Hyderabad, 500 001, India

SO Proceedings - Indian Academy of Sciences, Chemical Sciences (1991), 103(4), 549-56

CODEN: PIAADM; ISSN: 0253-4134

DT Journal

LA English

OS CASREACT 115:207264

AB 2-HOC6H4CO2CH2CH(OH)CH2O2CCMe:CH2 (I) and its derivs. (Me, methoxy, Ac, thio, amino, chloro, and bromo) were prepared and characterized by elemental

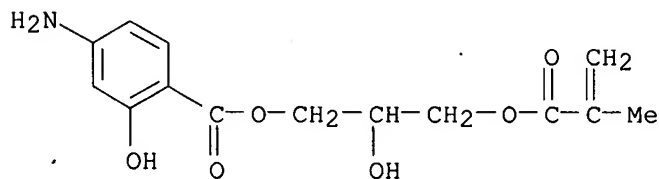
anal., mass, IR, and <sup>1</sup>H- and <sup>13</sup>C-NMR spectroscopic results. I formation was 2nd order overall, 1st order each in salicylic acid and glycidyl methacrylate. A structural change (substituent change) in the salicylic acid changed its reactivity during I formation. Second-order rate consts. increase in the order 5-bromo < 5-chloro < Ac < H < thio < 4-amino < 4-Me < 4-chloro. Hammett's plot indicated a rho (p) value of 0.43. Deviation in the case of p-chloro substituent was explained in terms of resonance-interaction energy (ΔΔG) parameters. The effective sigma (.hivin.σ) value of p-chloro was 0.86, with ΔΔGp 1.274 cal/mol. The isokinetic temperature (β) is far below the exptl. temperature range (325-355 K), indicating the importance of entropy factors in controlling the reaction.

IT 136910-45-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 136910-45-7 CAPLUS

CN Benzoic acid, 4-amino-2-hydroxy-, 2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:460785 CAPLUS

DN 115:60785

TI Developer for electrostatography

IN Tsubushi, Kazuo; Kuramoto, Shinichi; Umemura, Kazuhiko; Takahashi, Toshihiko; Uematsu, Hidemi

PA Ricoh Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02184865	A	19900719	JP 1989-5505	19890112
	JP 2849105	B2	19990120		
PRAI	JP 1989-5505		19890112		

AB The title developer contains a copolymer based on a monomer-containing dialkylaminobenzoic acid ester residue(s) or dialkylaminophthalic acid ester residue(s) and some other monomer. The developer (i.e. toner) gives copies with improved d., resolution, copy fixability, etc.

IT 135020-48-3D, copolymer with vinyl monomer

RL: USES (Uses)

(electrophotog. toner using)

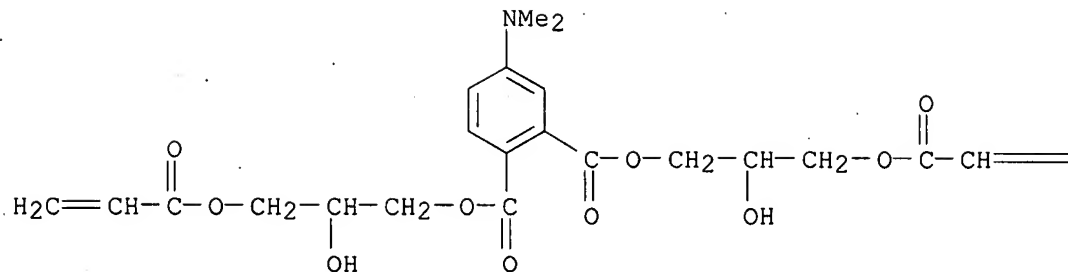
RN 135020-48-3 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(dimethylamino)-, bis[2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl] ester, polymer with butyl 2-methyl-2-propenoate and ethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

CM 1

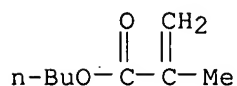
CRN 135020-47-2

CMF C22 H27 N O10

=CH<sub>2</sub>

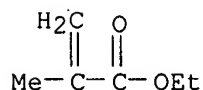
CM 2

CRN 97-88-1  
CMF C8 H14 O2



CM 3

CRN 97-63-2  
CMF C6 H10 O2



L3 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1989:423509 CAPLUS  
 DN 111:23509  
 TI Substituted 3-(4-nitrophenoxy)pyrazoles, their herbicidal use and  
 compositions, and processes and intermediates for their preparation  
 IN Moedritzer, Kurt; Lee, Len Fang; Rogers, Michael David; Anderson, Dennis  
 Keith; Singh, Rajendra Kumar; Gaede, Bruce John; Torrence, Lisa Louise  
 PA Monsanto Co., USA  
 SO Eur. Pat. Appl., 338 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1

PATENT NO.

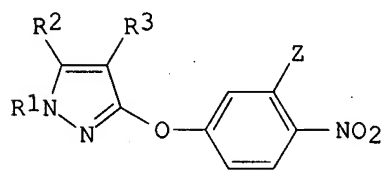
KIND

DATE

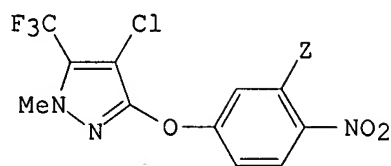
APPLICATION NO.

DATE

PI	EP 295233	A2	19881214	EP 1988-870104	19880607
	EP 295233	A3	19890315		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4855442	A	19890808	US 1988-175461	19880413
	US 4948902	A	19900814	US 1988-175462	19880413
	AU 8817450	A	19881208	AU 1988-17450	19880607
	AU 607225	B2	19910228		
	DK 8803086	A	19881209	DK 1988-3086	19880607
	FI 8802680	A	19881209	FI 1988-2680	19880607
	NO 8802509	A	19881209	NO 1988-2509	19880607
	NO 169387	B	19920309		
	NO 169387	C	19920617		
	BR 8802760	A	19881227	BR 1988-2760	19880607
	JP 01025764	A	19890127	JP 1988-140361	19880607
	JP 05075746	B	19931021		
	CN 1033457	A	19890621	CN 1988-103374	19880607
	CN 1021191	B	19930616		
	ZA 8804050	A	19900228	ZA 1988-4050	19880607
	HU 52063	A2	19900628	HU 1988-2946	19880607
	HU 204259	B	19911230		
	DD 289461	A5	19910502	DD 1988-316491	19880607
	PL 156831	B1	19920430	PL 1988-279591	19880607
	PL 156730	B1	19920430	PL 1988-279592	19880607
	PL 157154	B1	19920529	PL 1988-272883	19880607
	NO 8900595	A	19881209	NO 1989-595	19890210
	NO 170276	B	19920622		
	NO 170276	C	19920930		
	NO 8900596	A	19881209	NO 1989-596	19890210
	US 4964895	A	19901023	US 1990-471686	19900130
PRAI	US 1987-59431	A	19870608		
	US 1987-59712	A	19870608		
	US 1988-175460	A	19880413		
	US 1988-175461	A	19880413		
	US 1988-175462	A	19880413		
	US 1988-175463	A	19880413		
	NO 1988-2509	A1	19880607		
OS	CASREACT 111:23509; MARPAT 111:23509				
GI					



I



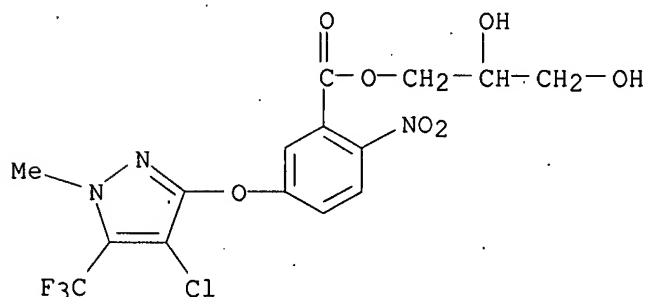
II

AB Title compds. I [R1 = Me, Et, halomethyl, haloethyl; R2 = Cl, cyano, halomethyl, haloethyl, MeS, EtS, MeS(O), EtS(O), MeS(O)2, EtS(O)2, MeOCH2; R3 = H, halo, NO2; Z = H, substituent of mol. weight ≤300] are prepared as herbicides. 3-Fluoroacetophenone underwent nitration by fuming HNO3 in the 6-position, followed by condensation with 5-trifluoromethyl-4-chloro-3-hydroxy-1-methylpyrazole to give (trifluoromethyl)chloro(nitrophenoxy)methylpyrazole II (Z = Ac). This underwent oximation by NH2OH.HCl, followed by etherification of the oxime with BrCH2CO2Me, to give II (Z = MeOCOCH2ON:CMc) (III). At 11.21 kg/ha postemergence, III gave 100% control of 9/10 tested weeds, including barnyardgrass, velvetleaf, and Pennsylvania smartweed.

IT 121303-65-9P

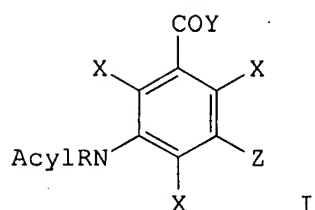
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as herbicide)  
 RN 121303-65-9 CAPLUS  
 CN Benzoic acid, 5-[[4-chloro-1-methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]oxy]-2-nitro-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1989:192447 CAPLUS  
 DN 110:192447  
 TI Preparation of 5-acylamino-2,4,6-triiodo- or tribromobenzoic acid derivatives, useful as radiologic contrast imaging components  
 IN Felder, Ernest; Musu, Carlo; Fumagalli, Luciano; Uggeri, Fulvio  
 PA Bracco Industria Chimica S.p.A., Italy  
 SO PCT Int. Appl., 70 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8809328	A1	19881201	WO 1988-EP453	19880520
	W: AU, BB, BG, SD, SU, US				
	RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	AU 8817978	A	19881221	AU 1988-17978	19880520
	AU 618535	B2	19920102		
	ZA 8803610	A	19890125	ZA 1988-3610	19880520
	ES 2006951	A6	19890516	ES 1988-1607	19880520
	EP 365541	A1	19900502	EP 1988-904526	19880520
	EP 365541	B1	19920812		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 02503556	T	19901025	JP 1988-504455	19880520
	JP 2585087	B2	19970226		
	AT 79368	T	19920815	AT 1988-904526	19880520
	CA 1327600	C	19940308	CA 1988-567436	19880520
	IL 86450	A	19940530	IL 1988-86450	19880520
	US 5066823	A	19911119	US 1989-424216	19891010
PRAI	IT 1987-20647	A	19870522		
	IT 1988-47935	A	19880510		
	EP 1988-904526	A	19880520		
	WO 1988-EP453	A	19880520		
OS	MARPAT 110:192447				
GI					



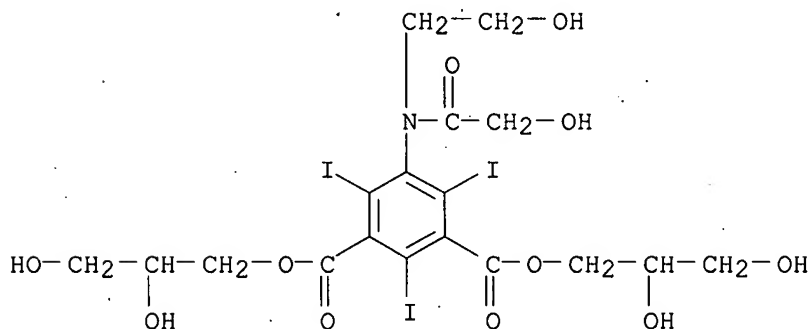
AB Title compds. I (X = Br, iodo; acyl = C2-6 hydroxyalkanoyl, alkoxyalkanoyl, alkoxyhydroxyalkanoyl, (un)substituted C2-4 alkanoyl; R = H, C1-6 alkyl, hydroxyalkyl, alkoxyalkyl, alkoxyhydroxyalkyl, H(OCH<sub>2</sub>CH<sub>2</sub>)<sub>2-5</sub>, Me(OCH<sub>2</sub>CH<sub>2</sub>)<sub>2-4</sub>, Et(OCH<sub>2</sub>CH<sub>2</sub>)<sub>2-4</sub>, alkylene analog of I; Y = HO, alkoxy, hydroxyalkoxy, alkylamino, etc.; Z = COY, hydroxyalkylaminocarbonyl, C2-5 acylamino, hydroxyacylamino, N-alkylacylamino, N-hydroxyalkylacylamino, acylaminomethyl), components of contrast agents in radiol. (no data) are prepared S-5-(1-Methylaminocarbonylethoxy)-2,4,6-triiodobis(1,3-dihydroxyisopropyl)isophthalamide in DMF was reacted with MeONa/MeOH at room temperature to give 70.4% I [Y = (HOCH<sub>2</sub>)<sub>2</sub>CHNH, Z = (HOCH<sub>2</sub>)<sub>2</sub>CHNHCO, acyl = MeCH(OH)COCH<sub>2</sub>, R = H, X = iodo].

IT 120396-61-4P 120396-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as radiocontrast agent)

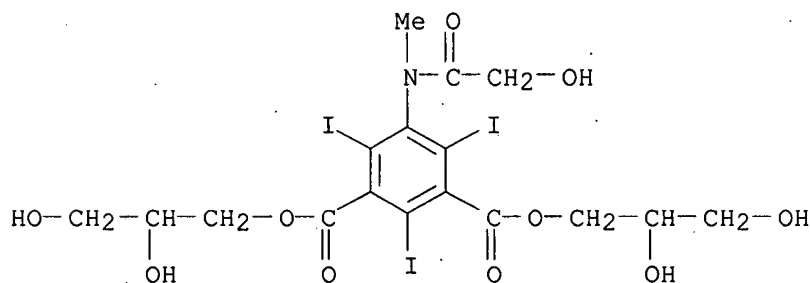
RN 120396-61-4 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[(hydroxyacetyl)(2-hydroxyethyl)amino]-2,4,6-triiodo-, bis(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)

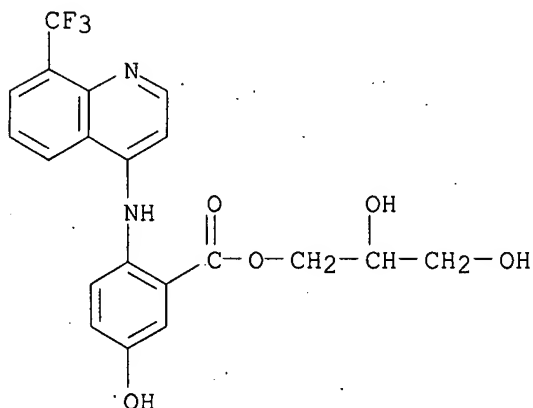


RN 120396-63-6 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[(hydroxyacetyl)methylamino]-2,4,6-triiodo-, bis(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)



DN 110:127904  
 TI Simultaneous determination of plasma floctafenin and its major metabolites by high-performance liquid chromatography: preliminary observations in children  
 AU Nicot, G.; Lachatre, G.; Terrier, G.; Gonnet, C.; Rocca, J. L.; Desroches, R.; Lansade, A.  
 CS Cent. Hosp. Reg., Univ. Hop. Dupuytren, Limoges, 87042, Fr.  
 SO Therapeutic Drug Monitoring (1989), 11(1), 67-72  
 CODEN: TDMODV; ISSN: 0163-4356  
 DT Journal  
 LA English  
 AB An isocratic reversed-phase ion-pair liquid chromatog. with UV detection at 350 nm for the determination in human plasma of floctafenin (F) and its 3 main metabolites [floctafenic acid (FA), hydroxyfloctafenin (HOF), and hydroxyfloctafenic acid (HOFA)] is reported. Analytes and internal standard were extracted from acidified plasma into EtOAc, and this organic phase was evaporated to dryness. This extraction yielded plasma drug recoveries of >72%. With 1 mL of plasma, the lower quantification limit was 0.05 µg/mL with excellent linearity up to 0.8 µg/mL for HOF and HOFA and up to 4.0 µg/mL for F and FA. The reproducibility and the selectivity of the method in the presence of several drugs thought likely to be administered in conjunction with F were demonstrated. This method was successfully applied to a pharmacokinetic study with a single 10-mg/kg oral dose in children.  
 IT 56047-11-1  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, as floctafenin metabolite, in blood of children by HPLC)  
 RN 56047-11-1 CAPLUS  
 CN Benzoic acid, 5-hydroxy-2-[[8-(trifluoromethyl)-4-quinolinyl]amino]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

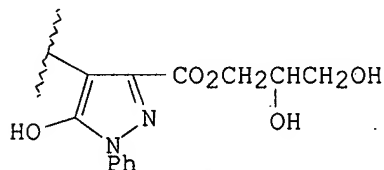
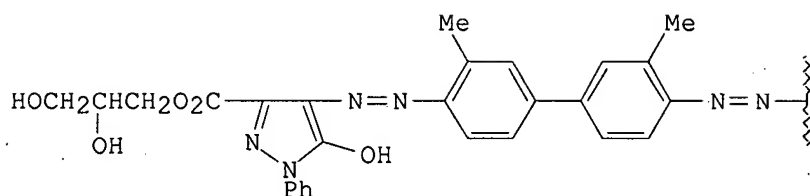


L3 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1988:530818 CAPLUS  
 DN 109:130818  
 TI Alcohol-soluble dye compositions  
 IN Ono, Takashi; Ikegami, Akiko  
 PA Orient Chemical Industries, Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63075068	A	19880405	JP 1986-221165	19860918

JP 06094546  
 PRAI JP 1986-221165  
 OS MARPAT 109:130818  
 GI

B 19941124  
 19860918



I

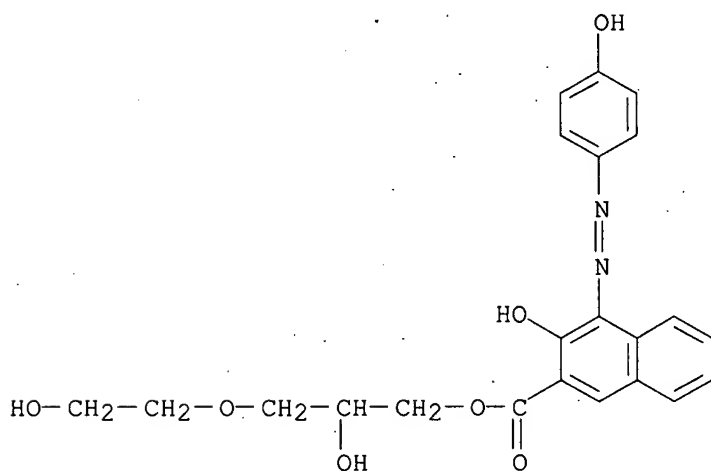
AB Dye compns., soluble in lower alcs. such as PrOH, BuOH, and propylene glycol monoalkyl ethers and useful for marking inks, comprise reaction mixts. obtained by treating dyes or their precursors containing active H connected to N or O and no other type of active H with epoxy compds. and converting the precursors to dyes. The reaction mixts. may contain compds.  $\text{Dm}[\text{CH}_2\text{CH}(\text{OH})\text{R}]_n$  [D = dye residue; R = C1-4 alkyl,  $\text{CH}_2\text{OR}_1$ ;  $\text{R}_1$  = H, C1-5 alkyl, C1-5 alkenyl, (meth)acryloyl,  $\text{CH}_2\text{CH}_2\text{CH}_2\text{Si}(\text{OMe})_3$ , polyol residue with mol. weight  $\leq 300$ ; m = 1-2; n = 1-4]. Thus, 0.2 mol 1-phenyl-3-carboxy-5-pyrazolone was treated with 0.6 mol glycidol and triethanolamine (catalyst) in  $\text{H}_2\text{O}$  at  $80-85^\circ$  and the product was coupled with 0.1 mol diazotized o-tolidine at  $10-15^\circ$  to give dye I. A 20% PrOH solution of I was stable when kept at  $-5$  or  $+60^\circ$  for 3 mo.

IT 116429-92-6P

RL: IMF (Industrial manufacture); PREP (Preparation)  
 (preparation of, alc.-soluble, for marking inks)

RN 116429-92-6 CAPLUS

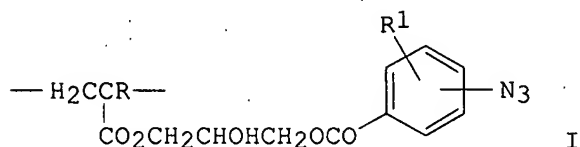
CN 2-Naphthalenecarboxylic acid, 3-hydroxy-4-[(4-hydroxyphenyl)azo]-,  
 2-hydroxy-3-(2-hydroxyethoxy)propyl ester (9CI) (CA INDEX NAME)





AN 1987:468173 CAPLUS  
 DN 107:68173  
 TI Negative-working photoresist  
 IN Goto, Yoshitaka; Yazawa, Toshiya; Fujii, Kenichi; Yamada, Eiichi  
 PA Nippon Oils & Fats Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61239245	A	19861024	JP 1985-80090	19850417
PRAI	JP 1985-80090		19850417		
GI					



AB The photosensitive component of the photoresist is a polymer having mol. weight  $\geq 5000$  and repeating units I ( $R = H$ , C1-2 alkyl;  $R1 = H$ , C1-3 alkyl, C1-3 alkoxy). The polymer has high photosensitivity and acid resistance and is storage stable. Thus, 2-hydroxy-3-azidobenzoyloxypropyl methacrylate 45, Et acrylate 30, benzyl methacrylate 25, tert-butyl 2-ethylperoxyhexanoate 1 parts and MEK were made to react at  $80^\circ$  for 5 h to give a polymer having mol. weight 75,000 after purification A

solution

containing the polymer and 5-nitroacenaphthene (10% weight of the polymer) was used to form a  $2\text{-}\mu$  layer on a Cu substrate. The material was sensitometrically exposed to a Hg lamp, developed with trichloroethylene, and etched with  $\text{FeCl}_3$ . Sensitivity was much higher than controls using poly(vinyl cinnamate) with or without a sensitizer or a similar polymer but having mol. weight 3500. The controls also showed inferior stabilities.

IT 109180-29-2 109180-31-6

RL: TEM (Technical or engineered material use); USES (Uses)  
 (photoresist composition containing, for improved stability)

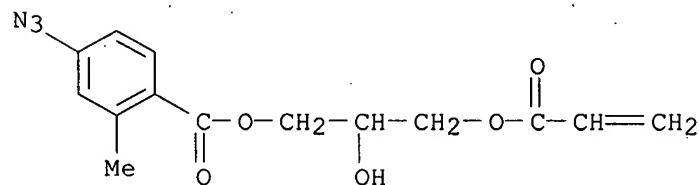
RN 109180-29-2 CAPLUS

CN 2-Butenedioic acid (2Z)-, dimethyl ester, polymer with ethenyl acetate and 2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl 4-azido-2-methylbenzoate.(9CI)  
 (CA INDEX NAME)

CM 1

CRN 109180-28-1

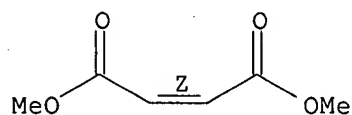
CMF C14 H15 N3 O5



CM 2

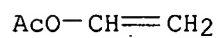
CRN 624-48-6  
CMF C6 H8 O4

Double bond geometry as shown.



CM 3

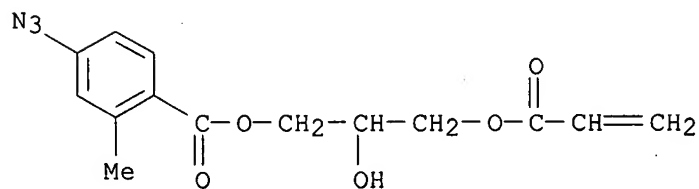
CRN 108-05-4  
CMF C4 H6 O2



RN 109180-31-6 CAPLUS  
CN Benzoic acid, 4-azido-2-methyl-, 2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl ester, polymer with ethenylbenzene and methyl 2-methyl-2-propenoate (9CI)  
(CA INDEX NAME)

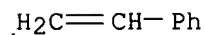
CM 1

CRN 109180-28-1  
CMF C14 H15 N3 O5



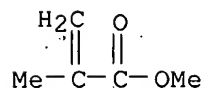
CM 2

CRN 100-42-5  
CMF C8 H8



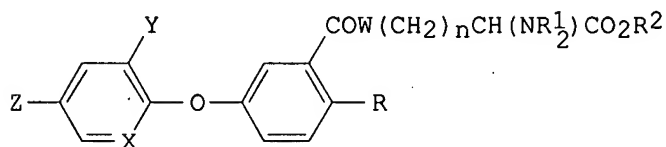
CM 3

CRN 80-62-6  
CMF C5 H8 O2



L3 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1986:621000 CAPLUS  
 DN 105:221000  
 TI Substituted aryloxybenzoyl amino acid herbicides and methods of use  
 IN Nagubandi, Sreeramulu  
 PA Stauffer Chemical Co., USA  
 SO U.S., 6 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4602946	A	19860729	US 1985-704815	19850225
PRAI	US 1985-704815		19850225		
OS	MARPAT 105:221000				
GI					

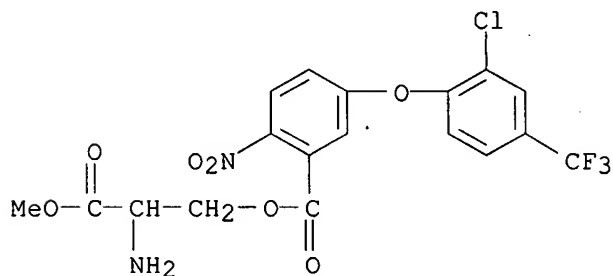


I

AB The title compound I (R = NO<sub>2</sub>, H, halo; R<sub>1</sub> = H, C1-6 alkyl, SCCl<sub>3</sub> etc.; R<sub>2</sub> = C1-8 alkyl, H, aryl, Mg, Ca, Ba, Fe, Cu, Zn, etc.; n = 1-4; W = O, S, NH; X = CH, N; Y = Cl, Br, F, iodo, Me, H, CN; Z = H, Cl, Br, iodo, F or CHmF<sub>3-m</sub>; m = 0-3) are prepared as herbicides. Thus, 79.0 g 2-nitro-5-[(2-chloro-4-trifluoromethyl)phenoxy]benzoyl chloride was reacted with 1.50 g DL-serine Me ester-HCl for 15-25 h to give I (R = NO<sub>2</sub>, R<sub>1</sub> = H, R<sub>2</sub> = Me, W = O, n = 1, X = CH, Y = Cl, Z = CF<sub>3</sub>) (II). Postemergence II, applied at 0.25 lb/acre, totally controlled foxtail (Setaria); hemp sesbania (Sesbania exaltata), nightshade (Solanum) and sorghum (Sorghum bicolor) in flats.

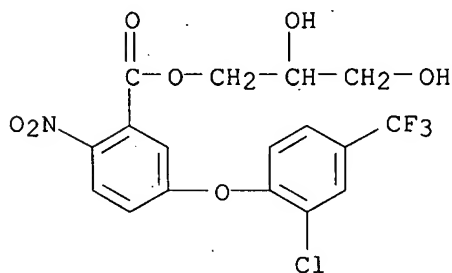
IT 105388-01-0P  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 105388-01-0 CAPLUS  
 CN Serine, methyl ester, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate (ester) (9CI) (CA INDEX NAME)



AN 1983:160411 CAPLUS  
 DN 98:160411  
 TI Phenoxybenzoates, compositions containing them and their use  
 IN Liu, Kou Chang; Brown, Michael J.  
 PA GAF Corp., USA  
 SO Eur. Pat. Appl., 96 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 66106	A1	19821208	EP 1982-103897	19820505
	R: BE, DE, FR, GB, IT				
	US 4435588	A	19840306	US 1981-283402	19810715
	US 4797505	A	19890110	US 1982-358974	19820317
	ZA 8203288	A	19831228	ZA 1982-3288	19820512
	ES 512427	A1	19830201	ES 1982-512427	19820521
	BR 8202970	A	19830503	BR 1982-2970	19820521
	JP 58010540	A	19830121	JP 1982-85702	19820522
	US 4568382	A	19860204	US 1983-557570	19831202
PRAI	US 1981-266675	A	19810522		
	US 1981-283402	A	19810715		
	US 1981-292320	A	19810812		
	US 1981-301664	A	19810914		
	US 1981-310663	A	19811013		
	US 1982-358974	A	19820317		
OS	CASREACT 98:160411; MARPAT 98:160411				
AB	Seventy herbicidal phenoxybenzoates 2,5-R(R1O)C6H3COR2 (I, R = NO2, cyano, amino; R1 = substituted Ph; R2 = esterified OH, SH, amino) were prepared by various methods. Thus, 448.1 g I [R = NO2, R1 = 2,4-Cl(F3C)C6H3, R2 = OH] was treated with 458 g SOCl2 to give 282.9 g acid chloride (II). II, (15 g) reacted with 10 g (HOCH2CH2S)2 to give 7.7 g I [R = NO2, R1 = 2,4-Cl(F3C)C6H3, R2 = OCH2CH2SSCH2CH2OH] (III). Applied both pre- and post-emergence, 10 lb III/acre gave complete kill of e.g. morning glory, with little effect on crop plants.				
IT	85300-90-9P RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and herbicidal activity of)				
RN	85300-90-9 CAPLUS				
CN	Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)				



L3 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1981:587045 CAPLUS  
 DN 95:187045  
 TI Benzoyl derivatives and their pharmaceutical use  
 IN Keck, Johannes; Krueger, Gerd; Pieper, Helmut; Noll, Klaus; Engelhardt,

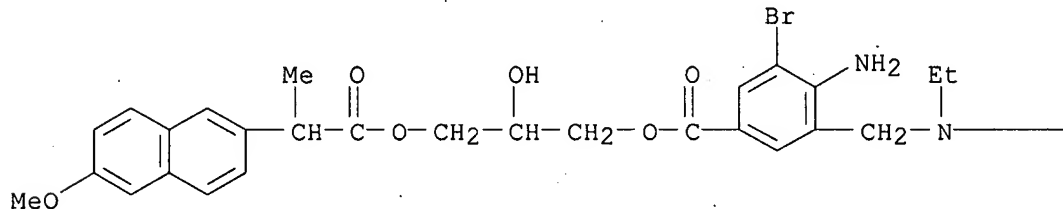
PA Guenther; Promberger, Norbert; Zimmermann, Rainer  
 SO Thoma, Dr. Karl, G.m.b.H., Fed. Rep. Ger.  
 Ger. Offen., 111 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 FAN.CNT 1

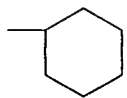
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2926472	A1	19810115	DE 1979-2926472	19790630
	EP 24282	A1	19810304	EP 1980-103099	19800604
	EP 24282	B1	19830518		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AT 3415	T	19830615	AT 1980-103099	19800604
	JP 56010155	A	19810202	JP 1980-78281	19800610
	US 4362738	A	19821207	US 1980-158587	19800611
	DK 8002794	A	19801231	DK 1980-2794	19800627
	FI 8002049	A	19801231	FI 1980-2049	19800627
	NO 8001931	A	19810102	NO 1980-1931	19800627
	AU 8059735	A	19810205	AU 1980-59735	19800627
	AU 538776	B2	19840830		
	ES 492845	A1	19811101	ES 1980-492845	19800627
	IL 60418	A	19840229	IL 1980-60418	19800627
	ZA 8003907	A	19820224	ZA 1980-3907	19800630
	CA 1140564	A1	19830201	CA 1980-355151	19800630
PRAI	DE 1979-2926472	A	19790630		
	EP 1980-103099	A	19800604		
OS	MARPAT 95:187045				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R, R1 = H, alkyl, optionally substituted Ph; RR1 =  
 alkylene, (CH2CH2)2N; R2 = H, F, Cl, Br; R3 = acyl; X = O, NH; X1 =  
 cycloalkylene, alkylene, carbalkoxy] were prepared Thus, II.HCl was stirred  
 with III overnight to give IV. IV had an ED35 = 84.7 mg/kg (s.c.) in the  
 carrageenin edema test.  
 IT 78436-58-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (deacetylation of)  
 RN 78436-58-5 CAPLUS  
 CN 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, 3-[[4-amino-3-bromo-5-  
 [(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester (9CI)  
 (CA INDEX NAME)

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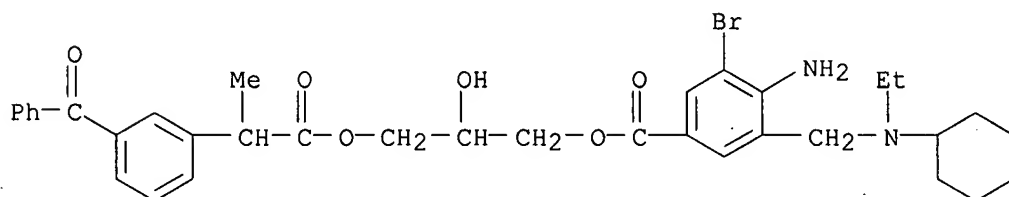


IT 78436-49-4P 78436-53-0P 78436-58-5P  
 78436-60-9P 78436-64-3P 78458-40-9P  
 78458-47-6P 78458-48-7P 78458-49-8P  
 78458-50-1P 78458-51-2P 78458-53-4P  
 78458-55-6P 78480-99-6P 78481-00-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 78436-49-4 CAPLUS

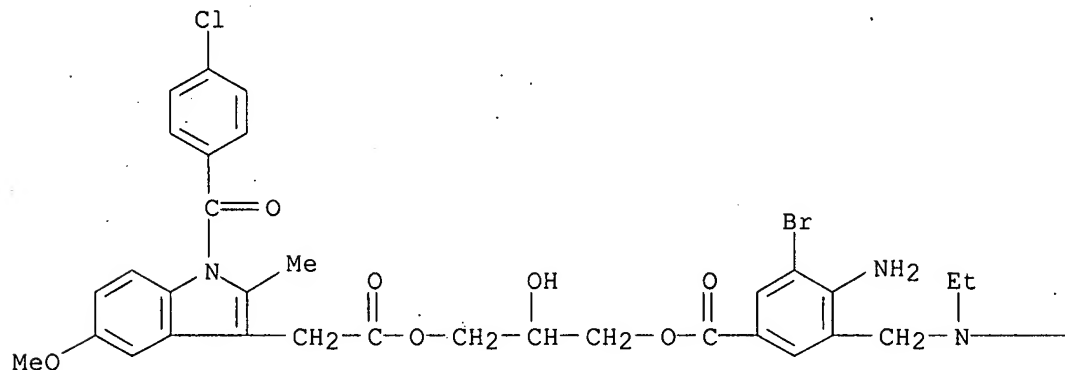
CN Benzeneacetic acid, 3-benzoyl- $\alpha$ -methyl-, 3-[[4-amino-3-bromo-5-  
 [(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester,  
 monohydrochloride (9CI) (CA INDEX NAME)

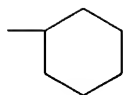


● HCl

RN 78436-53-0 CAPLUS

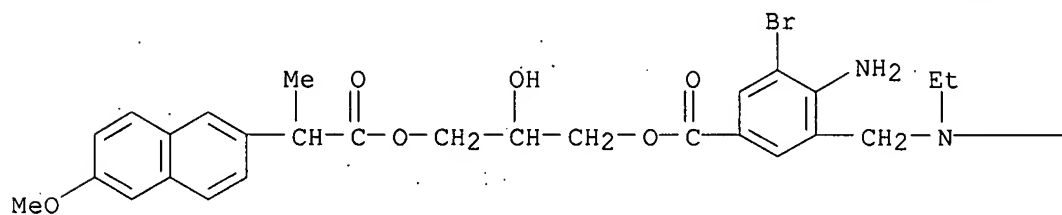
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-,  
 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-  
 hydroxypropyl ester (9CI) (CA INDEX NAME)



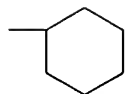


RN 78436-58-5 CAPLUS  
 CN 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, 3-[[4-amino-3-bromo-5-  
 [(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester (9CI)  
 (CA INDEX NAME)

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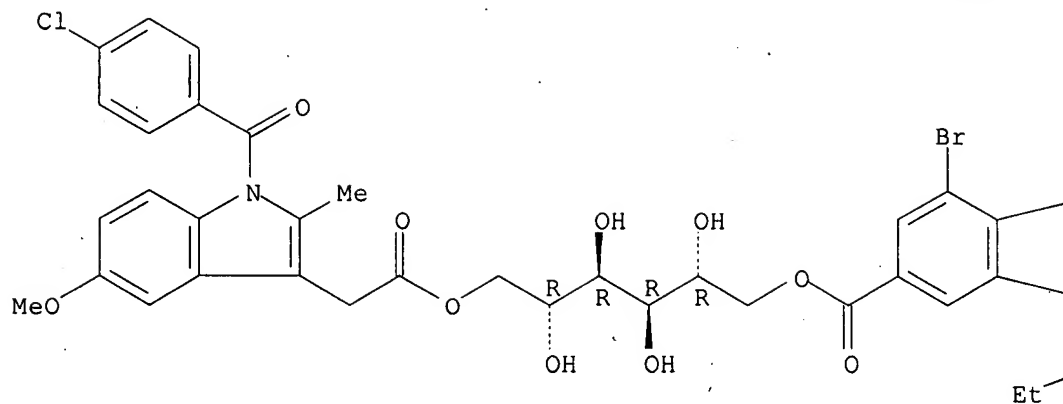


PAGE 1-B

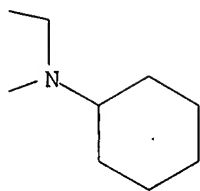


RN 78436-60-9 CAPLUS  
 CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate]  
 6-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetate] (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

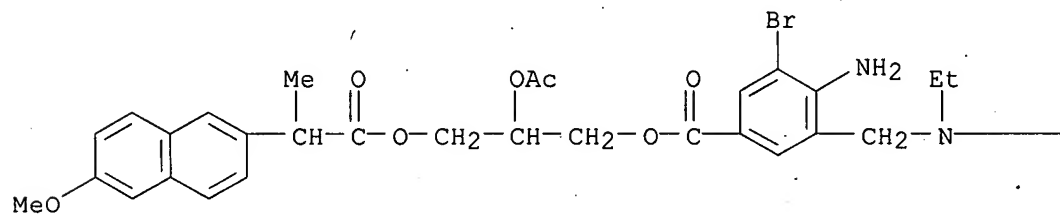


NH<sub>2</sub>



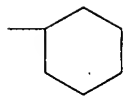
RN 78436-64-3 CAPLUS

CN 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, 2-(acetyloxy)-3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)



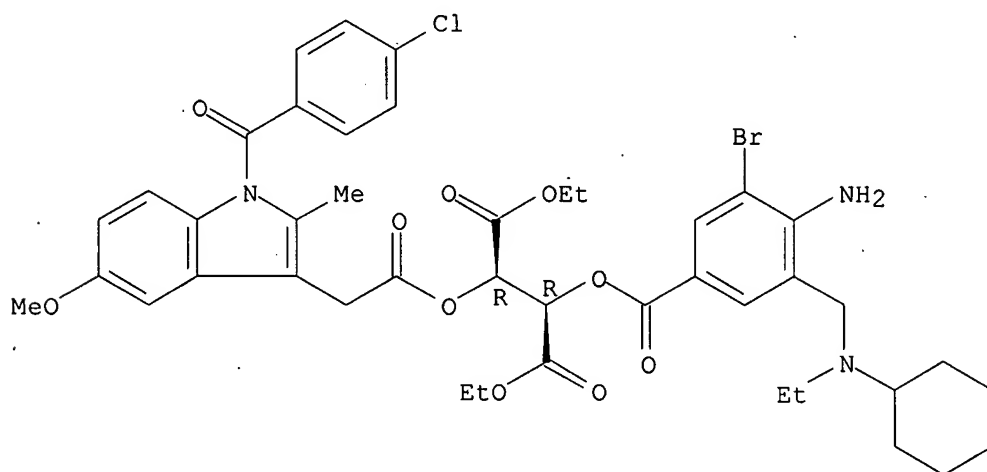
● HCl



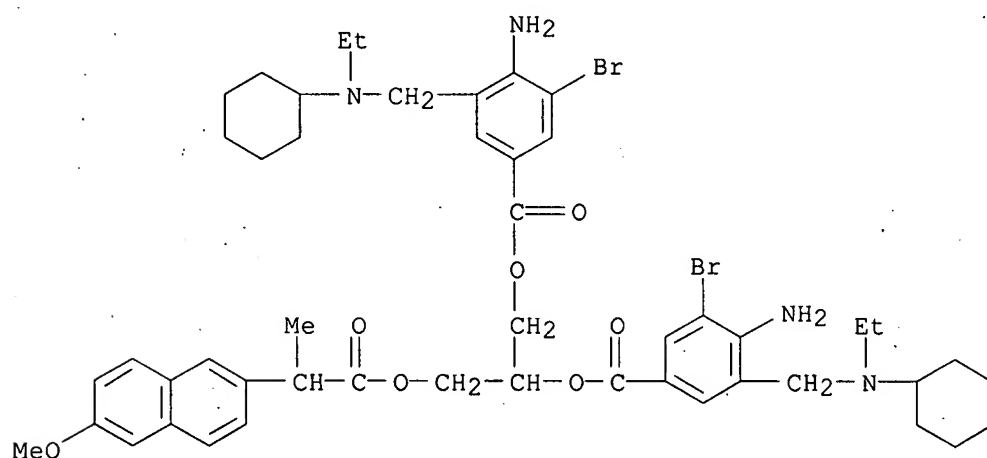


RN 78458-40-9 CAPLUS  
 CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-[[[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl]acetyl]oxy]-, diethyl ester, [R-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

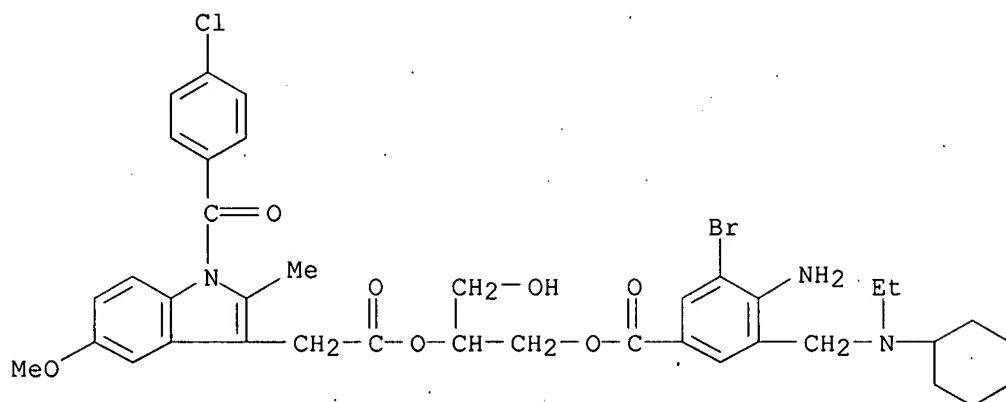


RN 78458-47-6 CAPLUS  
 CN 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, 2,3-bis[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]propyl ester (9CI) (CA INDEX NAME)



RN 78458-48-7 CAPLUS  
 CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-1-

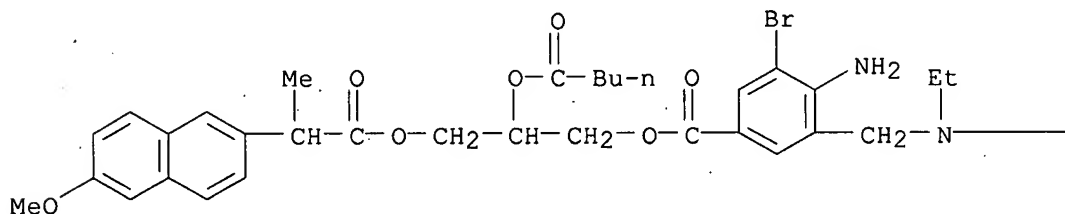
(hydroxymethyl)ethyl ester (9CI) (CA INDEX NAME)



RN 78458-49-8 CAPLUS

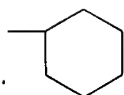
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxopentyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

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● HCl

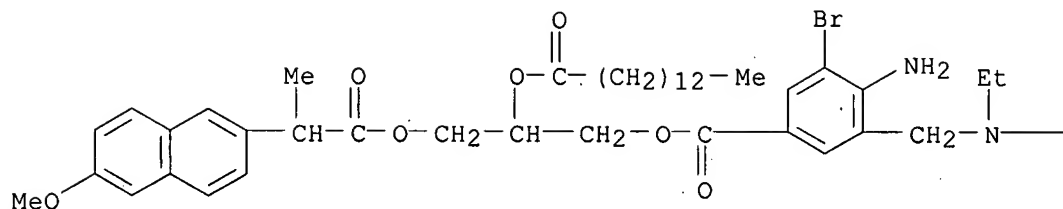
PAGE 1-B



RN 78458-50-1 CAPLUS

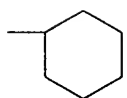
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxotetradecyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



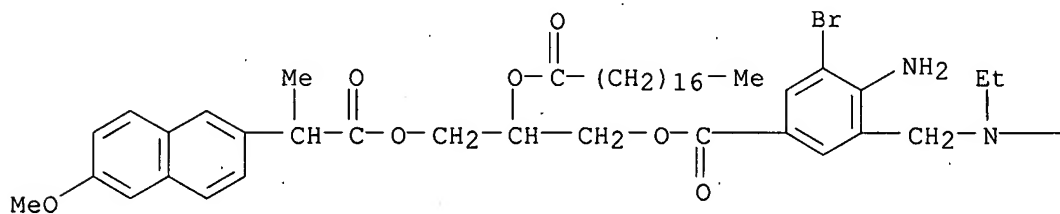
● HCl

PAGE 1-B



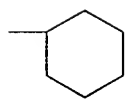
RN 78458-51-2 CAPLUS  
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxooctadecyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



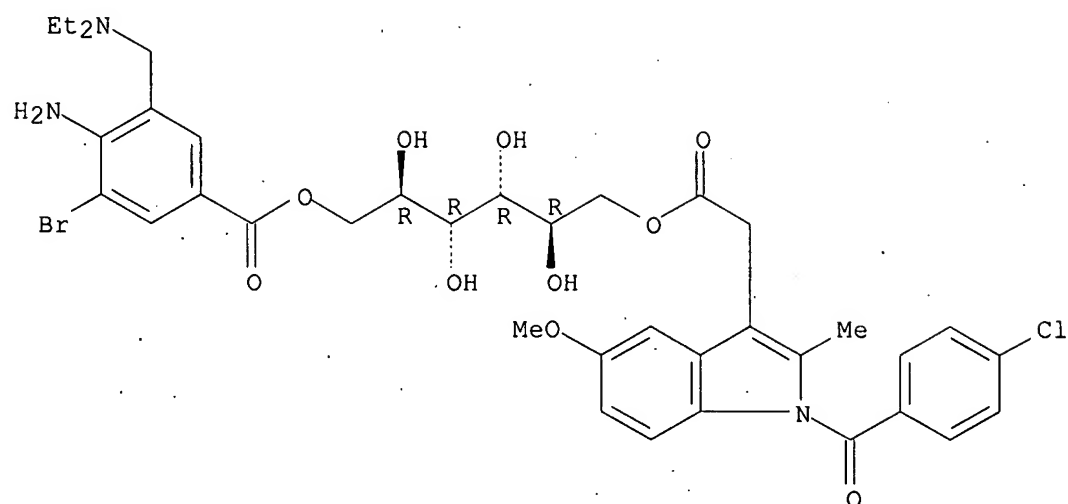
● HCl

PAGE 1-B



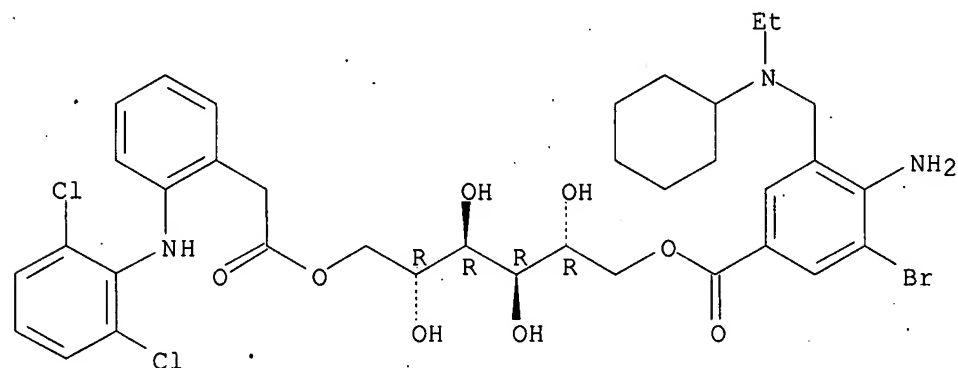
RN 78458-53-4 CAPLUS  
CN D-Mannitol, 1-[4-amino-3-bromo-5-[(diethylamino)methyl]benzoate] 6-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



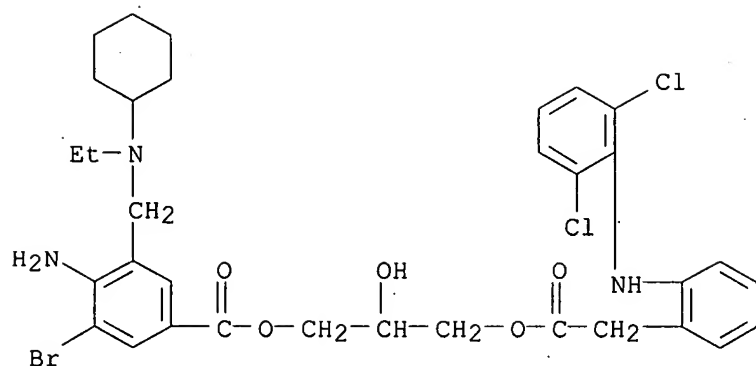
RN 78458-55-6 CAPLUS  
 CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate]  
 6-[2-[(2,6-dichlorophenyl)amino]benzeneacetate], monohydrochloride (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



● HCl

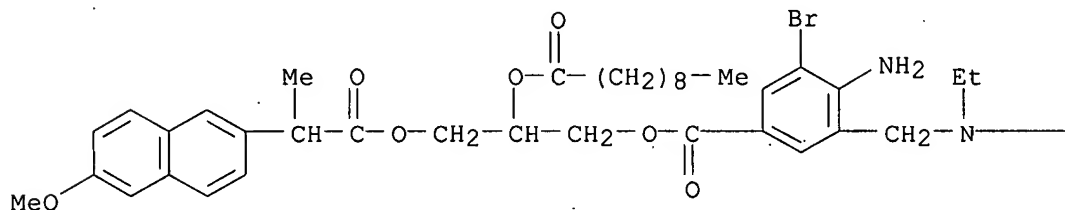
RN 78480-99-6 CAPLUS  
 CN Benzeneacetic acid, 2-[(2,6-dichlorophenyl)amino]-, 3-[[4-amino-3-bromo-5-  
 [(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester,  
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

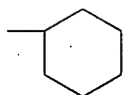
RN 78481-00-2 CAPLUS  
 CN 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxodecyl)oxy]propyl ester; monohydrochloride (9CI) (CA INDEX NAME)

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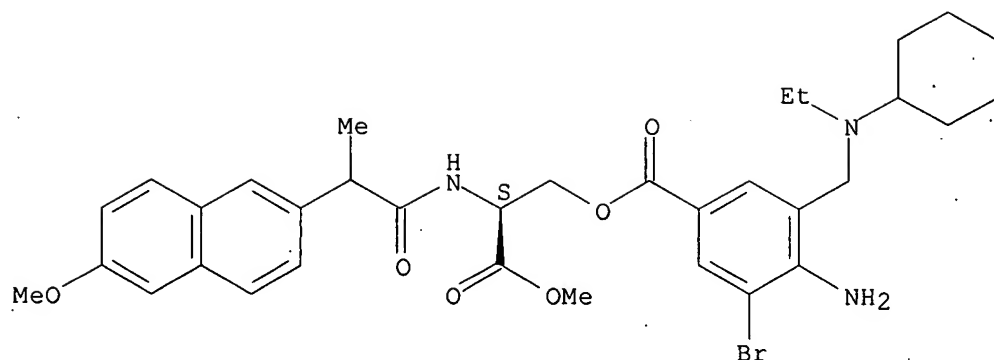
● HCl

PAGE 1-B



IT 78436-55-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with indoleacetic acid imidazolid)  
 RN 78436-55-2 CAPLUS  
 CN L-Serine, N-[2-(6-methoxy-2-naphthalenyl)-1-oxopropyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



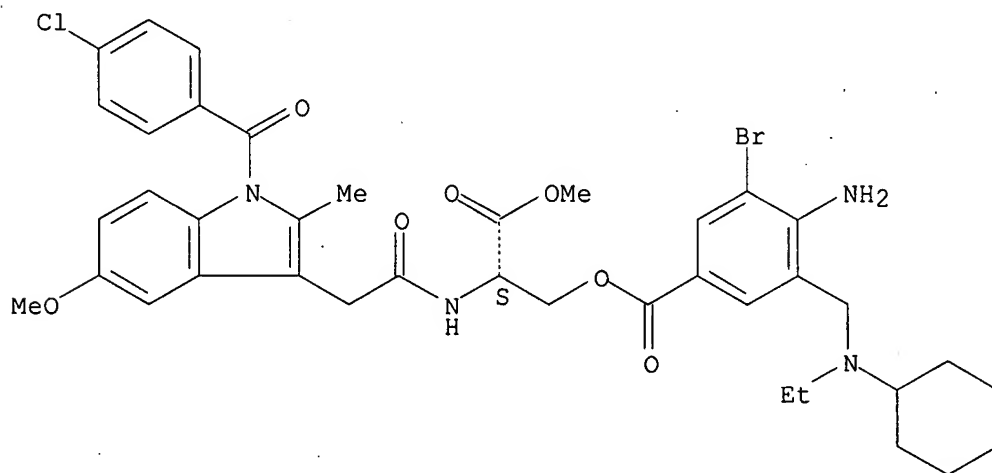
IT 78458-83-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with naphthaleneacetic acid imidazolidide)

RN 78458-83-0 CAPLUS

CN L-Serine, N-[[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl]acetyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

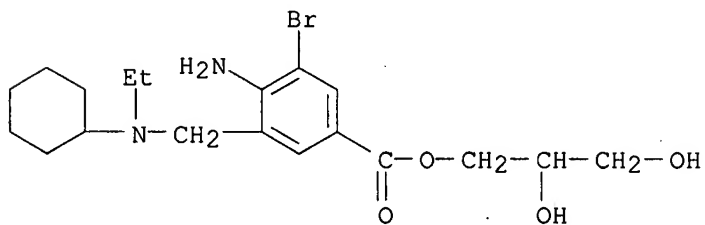


IT 78412-77-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetic acid imidazolidide derivative)

RN 78412-77-8 CAPLUS

CN Benzoic acid, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

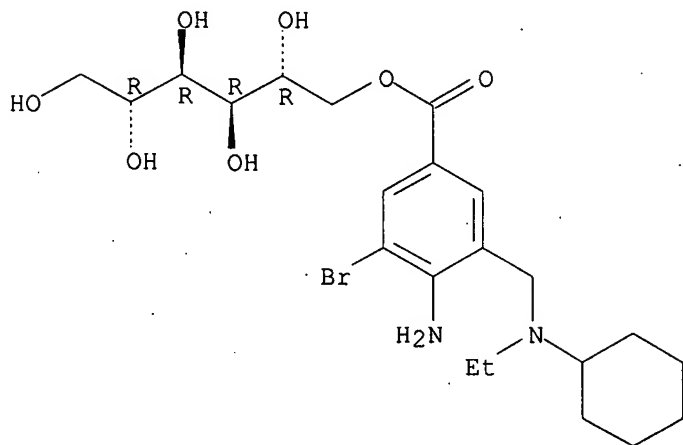


IT 78458-54-5

RL: RCT (Reactant); RACT (Reactant or reagent)

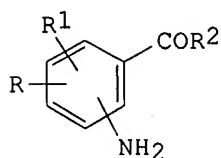
(reaction of, with phenylaminophenylacetic acid)  
 RN 78458-54-5 CAPLUS  
 CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate]  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

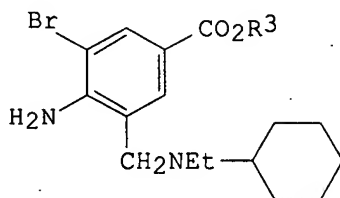


L3 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1981:461792 CAPLUS  
 DN 95:61792  
 TI Aminobenzoic acid derivatives for use as pharmaceuticals or intermediate products  
 IN Noll, Klaus; Keck, Johannes; Pieper, Helmut; Krueger, Gerd; Ballhause, Helmut; Bauer, Eckhart  
 PA Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.  
 SO Ger. Offen., 60 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2926471	A1	19810115	DE 1979-2926471	19790630
	JP 56010154	A	19810202	JP 1980-78280	19800610
	AT 8003063	A	19820715	AT 1980-3063	19800611
	AT 370085	B	19830225		
	DK 8002793	A	19801231	DK 1980-2793	19800627
	FI 8002048	A	19801231	FI 1980-2048	19800627
	NO 8001930	A	19810102	NO 1980-1930	19800627
	ES 492843	A1	19811116	ES 1980-492843	19800627
	CA 1140934	A1	19830208	CA 1980-355165	19800630
PRAI	DE 1979-2926471	A	19790630		
OS	MARPAT 95:61792				
GI					



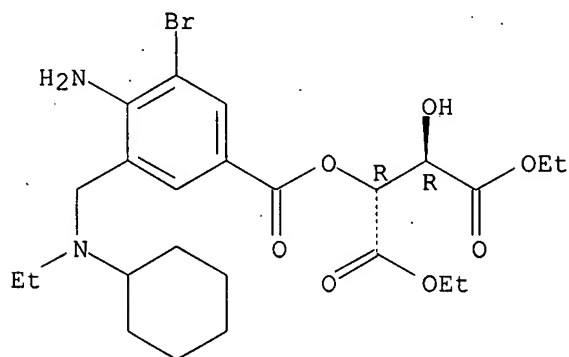
I



II

- AB Aminobenzoates I (R = aminomethyl; R1 = H, F, Cl, Br; R2 = esterified OH, substituted NH2) were prepared. Thus II (R3 = Na) was treated with chloropropanediol to give II [R3 = CH2CH(OH)CH2OH] (III). At 100 mg/kg orally in rats III caused 89% inhibition of gastric erosion induced by EtOH.
- IT 78412-80-3  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (antiulcer activity of)
- RN 78412-80-3 CAPLUS
- CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-hydroxy-, diethyl ester, monohydrochloride, [R-(R\*,R\*)]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

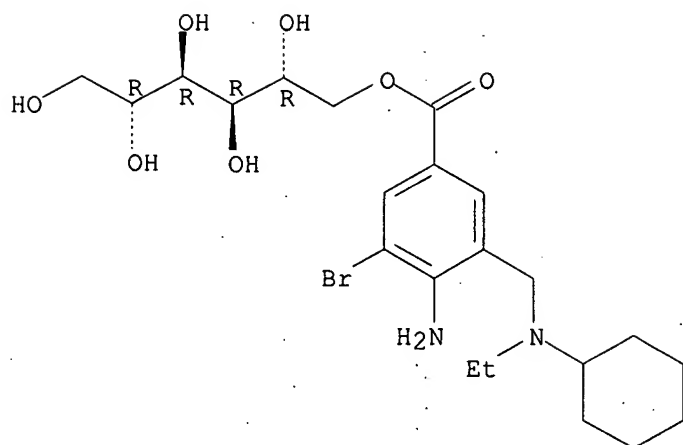


● HCl

- IT 78411-95-7P 78412-81-4P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation and antiulcer activity of)
- RN 78411-95-7 CAPLUS
- CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate], monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

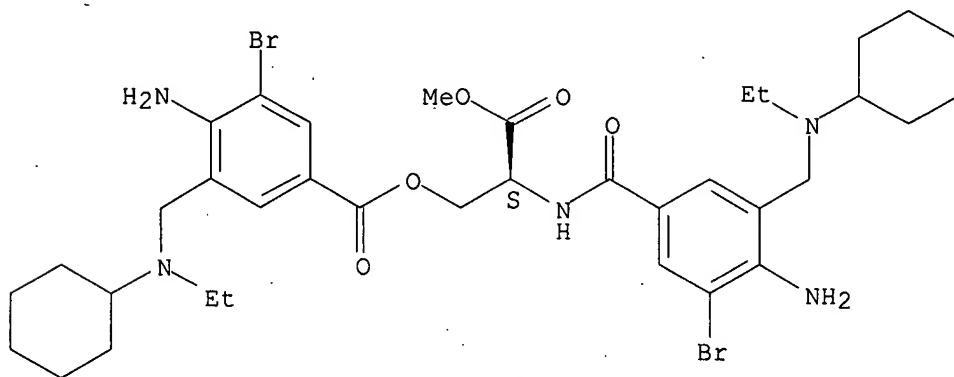




● HCl

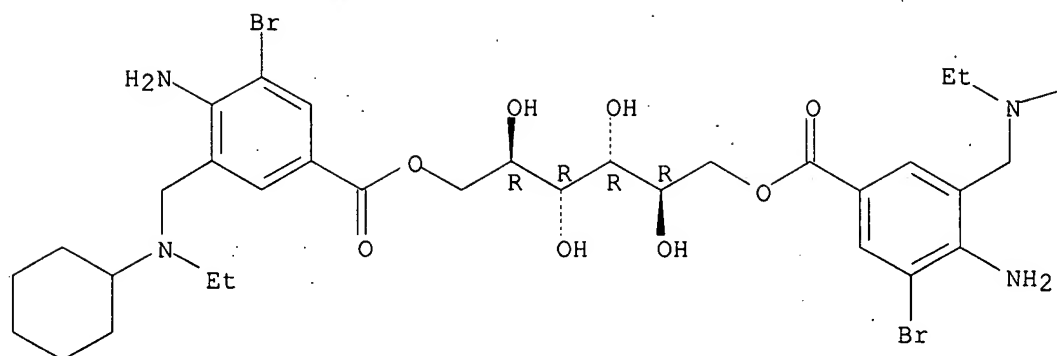
RN 78412-81-4 CAPLUS  
 CN L-Serine, N-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester). (9CI) (CA INDEX NAME)

Absolute stereochemistry.

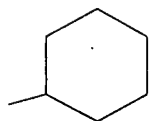


IT 78411-94-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)  
 RN 78411-94-6 CAPLUS  
 CN D-Mannitol, 1,6-bis[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate], dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl



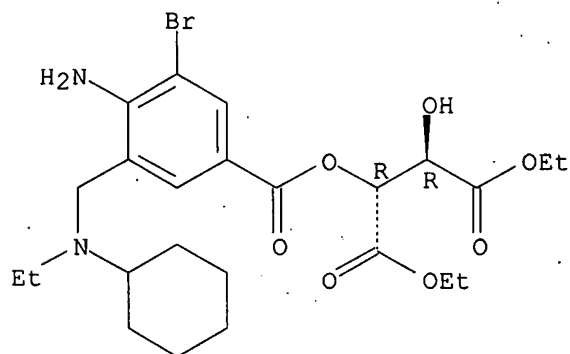
IT 78412-12-1P 78412-42-7P 78412-77-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 78412-12-1 CAPLUS

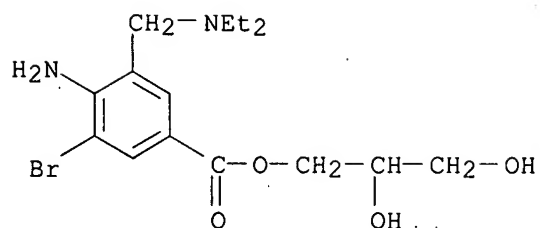
CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-hydroxy-, diethyl ester, [R-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

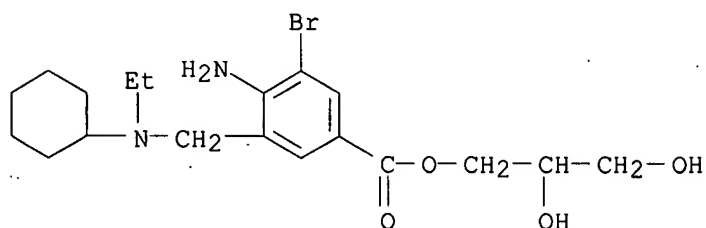


RN 78412-42-7 CAPLUS

CN Benzoic acid, 4-amino-3-bromo-5-[(diethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

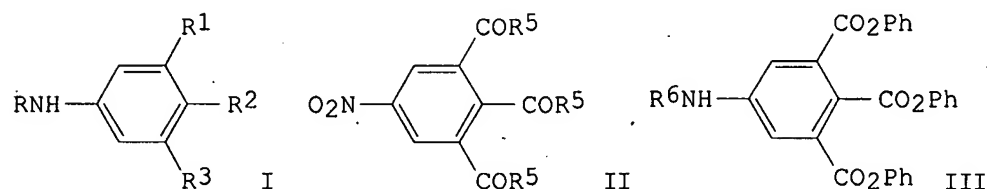


RN 78412-77-8 CAPLUS  
 CN Benzoic acid, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1981:442668 CAPLUS  
 DN 95:42668  
 TI 4-(Monoalkylamino)benzene polycarboxylic acids  
 IN Shepherd, Robert G.  
 PA American Cyanamid Co., USA  
 SO U.S., 8 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4245120	A	19810113	US 1977-836945	19770927
	US 4245119	A	19810113	US 1978-959537	19781113
PRAI	US 1977-836945	A3	19770927		
OS	MARPAT 95:42668				
GI					



AB Title compds. I [R = C8-19 alkyl; R1, R2, and R3 = H or CO2R4 (R4 = H, C1-4 alkyl, carboxalkyl, hydroxyalkyl dihydroxyalkyl, dialkylaminohydroxyalkyl, polymethyleneiminohydroxyalkyl, Ph, halophenyl, carboxyphenyl, CH2Ph, halobenzyl, carboxybenzyl, pyridylmethyl, halopyridylmethyl, carboxypyridylmethyl, 3-pyridyl, halo-3-pyridyl, carboxy-3-pyridyl, alkali metal cations, alkaline earth metal cations); only one member of R1, R2, or R2 can be H] were prepared as hypolipemics and antiatherosclerotic agents. Thus, 1,2,3-benzenetricarboxylic acid was

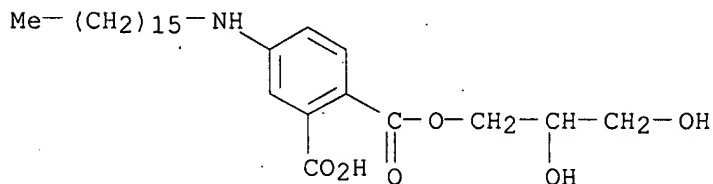
nitrated to give nitrobenzene II (R5 = OH), which was treated with SOCl<sub>2</sub> to give II (R5 = Cl), which was esterified with PhOH to give II (R5 = OPh). The latter was hydrogenated over Pd/C to give aminobenzenetricarboxylate III (R6 = H), which was alkylated with 1-bromohexadecane to give III (R6 = hexadecyl), which was saponified to give I (R = hexadecyl, R1-R3 = CO<sub>2</sub>H).

IT 78319-28-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 78319-28-5 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(hexadecylamino)-, 1-(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)



L3 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:220702 CAPLUS

DN 92:220702

TI X-ray contrast material

IN Felder, Ernst; Pitre, Davide

PA Bracco Industria Chimica S.p.A., Italy

SO Patentschrift (Switz.), 9 pp.

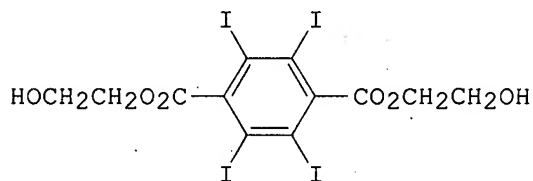
CODEN: SWXXAS

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CH 615344	A5	19800131	CH 1975-7800	19750616
PRAI	CH 1975-7800	A	19750616		
GI					



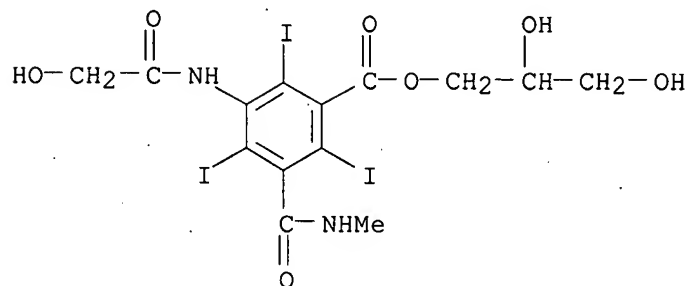
AB An x-ray contrast medium for the lymph system contains a micronized iodobenzoate in a protective colloid. Thus, 358 g micronized I [61838-98-0] was suspended in 370 mL 2% gelatin in 0.9% NaCl, to give a mixture containing 480 mg iodine/mL with a viscosity of 6.1 cP at 37°, pH 7.35, sedimentation quotient of 1 at 2 h and 0.97 at 24 h. The iodobenzoates rapidly cleared from the lymph system and do not cause inflammation. Enlargement of lymph nodes at the injection site is only 10-20%.

IT 73721-26-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 73721-26-3 CAPLUS

CN Benzoic acid, 3-[(hydroxyacetyl)amino]-2,4,6-triiodo-5-  
[(methylamino)carbonyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

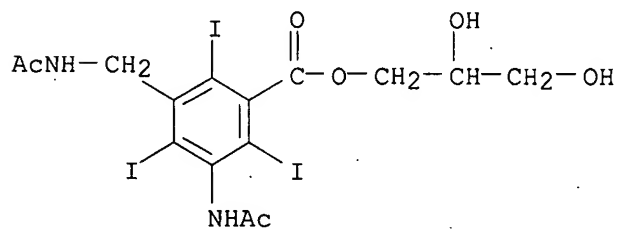


IT 67093-13-4

RL: BIOL (Biological study)  
(radiog. contrast media containing)

RN 67093-13-4 CAPLUS

CN Benzoic acid, 3-(acetylamino)-5-[(acetylamino)methyl]-2,4,6-triiodo-,  
2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:104420 CAPLUS

DN 92:104420

TI Mechanism of renal effects of large doses of glafenine in the rat

AU Peterfalvi, M.; Deraedt, R.; Pottier, J.; Vannier, B.; Boissier, J. R.

CS Cent. Rech. Roussel-Uclaf, Romainville, 93230, Fr.

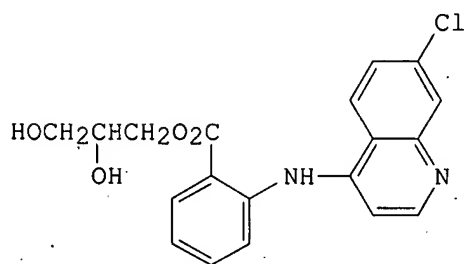
SO Therapie (1979), 34(3), 377-91

CODEN: THERAP; ISSN: 0040-5957

DT Journal

LA French

GI



I

AB In the rat, the oral LD50 of glafenine (I) [3820-67-5] is .apprx.2,300  
mg/kg. High oral doses, well above the pharmacol. active ones (2 to 10

mg/kg), induced reversible acute renal failure, the threshold dose being .apprx.200 mg/kg. The kidney damage is characterized by an increase of serum urea, intrarenal water retention and dilation and flattening of the epithelium of the renal tubules. I nephrotoxicity can be avoided by fractionation of the toxic dose in several administrations. The high doses also exerted an antidiuretic effect. The pathogenesis of this acute renal failure is characterized by early obstruction of the collecting tubules by deposits which are yellow colored due to accumulation of the I metabolite, hydroxyglafenine acid [72071-22-8]. Of the urinary metabolites of I only hydroxyglafenine acid was nephrotoxic by i.v. route.

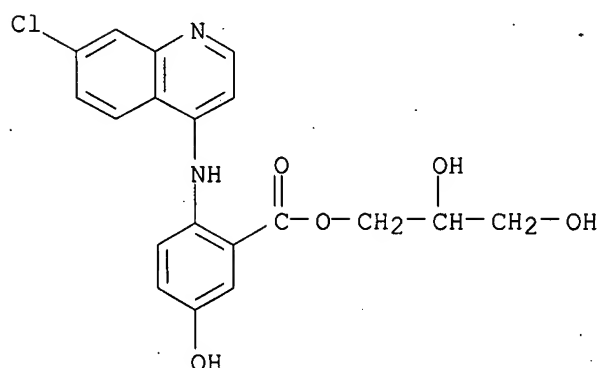
IT 72071-23-9

RL: BIOL (Biological study)

(as glafenine metabolite, toxicity in relation to)

RN 72071-23-9 CAPLUS

CN Benzoic acid, 2-[(7-chloro-4-quinolinyl)amino]-5-hydroxy-,  
2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:152 CAPLUS

DN 92:152

TI Biotransformations of glafenine in the rat and in man

AU Pottier, J.; Busigny, M.; Raynaud, J. P.

CS Cent. Rech. Roussel-Uclaf, Romainville, 93230, Fr.

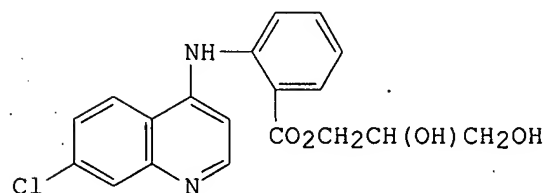
SO European Journal of Drug Metabolism and Pharmacokinetics (1979), 4(2),  
109-15

CODEN: EJDPD2; ISSN: 0398-7639

DT Journal

LA English

GI



I

AB The biotransformations of a therapeutic dose of the nonnarcotic analgesic glafenine (I) [3820-67-5], were studied in the rat and in man. In the rat, the ester bond was hydrolyzed to give glafenine acid [10440-42-3] the major metabolite excreted in the bile and urine. Two minor pathways were identified; hydroxylation of the benzene ring of I or glafenine acid para to the amino-substituent and oxidation of the quinoline N of glafenine acid,

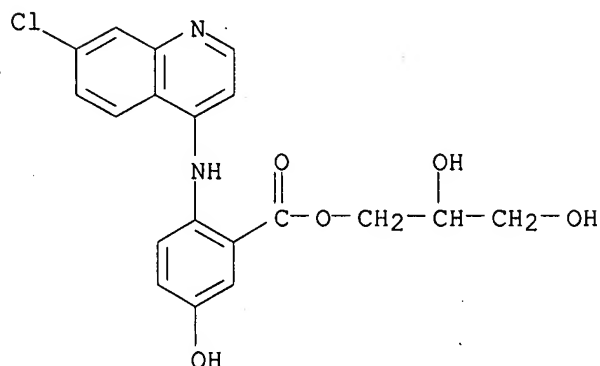
to its N-oxide. In vivo, this N-oxide was partly reduced to the parent compound Hydroxyglafenic acid [72071-22-8] was the product of both direct oxidation of glafenic acid and hydrolysis of hydroxyglafenine. The glyceric esters were conjugated as glucuronides and(or) sulfate esters and the carboxylic metabolites as acyl glucuronides. The analogous urinary excretion patterns in man and in the rat suggest a similarity in the biotransformations of I in these 2 species.

IT 72071-23-9

RL: BIOL (Biological study)  
(as glafenine metabolite)

RN 72071-23-9 CAPLUS

CN Benzoic acid, 2-[(7-chloro-4-quinolinyl)amino]-5-hydroxy-,  
2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:438776 CAPLUS

DN 89:38776

TI Radiopaque contrast media. XLV. Experimental lymphography with crystal suspensions

AU Felder, E.; Pitre, D.; Tirone, P.; Zingales, M. F.

CS Res. Lab., Bracco Ind. Chim. S.p.A., Milan, Italy

SO Farmaco, Edizione Scientifica (1978), 33(4), 302-14

CODEN: FRPSAX; ISSN: 0430-0920

DT Journal

LA English

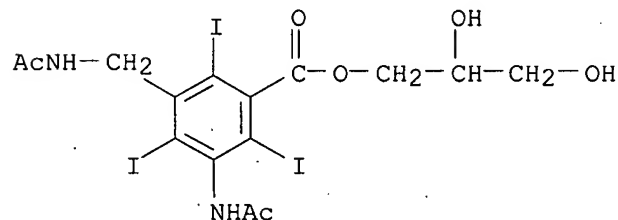
AB The preparation, properties, toxicity, and pharmacokinetics of iodomide and 2,3,5,6-tetraiodoterephthalic acid derivs. were presented, and their use in lymphog. was examined in dogs. The iodinated contrast media gave sharp image delineation, and had low viscosity and good miscibility for enhanced lymphatic uptake.

IT 67093-13-4

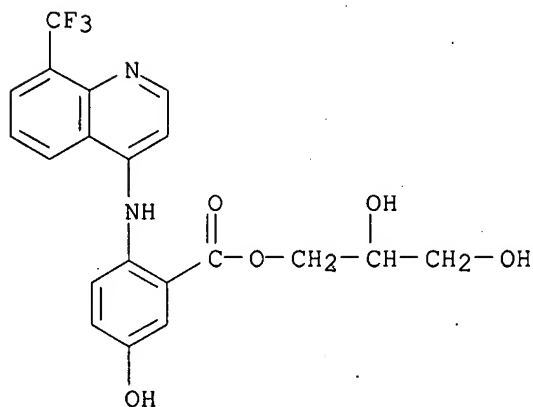
RL: BIOL (Biological study)  
(contrast media, for lymphog.)

RN 67093-13-4 CAPLUS

CN Benzoic acid, 3-(acetylamino)-5-[(acetylamino)methyl]-2,4,6-triiodo-,  
2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1975:471462 CAPLUS  
 DN 83:71462  
 TI Pharmacokinetic study of a peripheral analgesic, floctafenin, in man, mouse, rat, and dog  
 AU Pottier, J.; Busigny, M.; Raynaud, J. P.  
 CS Cent. Rech., Roussel-Uclaf, Romainville, Fr.  
 SO Drug Metabolism and Disposition (1975), 3(3), 133-47  
 CODEN: DMDSAI; ISSN: 0090-9556  
 DT Journal  
 LA English  
 GI For diagram(s), see printed CA Issue.  
 AB The pharmacokinetics of floctafenin (I) [23779-99-9] was studied in man, mice, rats, and dogs at pharmacol. doses. Its absorption, which was exclusively intestinal, was good in man and rodents, but only partial in dogs. Its high plasma clearance rate was primarily due to hepatic hydrolysis to floctafenic acid [36783-34-3], which was the main circulating product almost immediately following i.v. administration. This compound bound to 2 sets of binding sites in animal serum and human plasma with affinity consts. of  $107M^{-1}$  and  $105M^{-1}$  at  $4^{\circ}$  in all species except the dog, where binding was weaker. This binding was solely accounted for by albumin. Floctafenin, less protein-bound than floctafenic acid, diffused more widely into tissues, but very low quantities of the ester and virtually negligible quantities of the acid crossed the blood-brain barrier, indicating that their analgesic activity was exclusively peripheral. The elimination of floctafenin and its metabolites was practically complete in 24 hr. The main excretory route was via the bile, biliary excretion being largely predominant in dogs and rats, and somewhat less so in man and mice. There was no enterohepatic cycle of note. The main metabolite in both bile and urine was floctafenic acid. A secondary metabolic pathway, common to all species, led, by hydroxylation in the position para to the anthranilic nitrogen, to the corresponding phenols. All products in man and rats were excreted primarily in the form of ether and/or ester O-glucuronides.  
 IT 56047-11-1  
 RL: BIOL (Biological study)  
 (as floctafenin metabolite, species in relation to)  
 RN 56047-11-1 CAPLUS  
 CN Benzoic acid, 5-hydroxy-2-[[8-(trifluoromethyl)-4-quinolinyl]amino]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1965:499399 CAPLUS  
 DN 63:99399



OREF 63:18367f-g

TI Purity of terephthalic acid for conversion into poly(ethylene terephthalate)

PA Toyo Rayon Co., Ltd.

SO 4 pp.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1000045		19650804	GB 1962-12800	19620403
PRAI	JP		19610417		

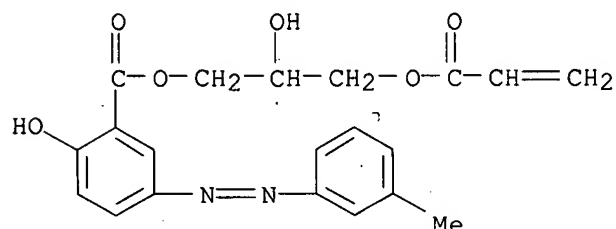
AB The purity of terephthalic acid (I) to be esterified directly with ethylene glycol can be tested by a light transmittance method. Thus, the light transmittance of 7.5 g. I in 50 ml. 2N KOH is compared with the transmittance of a 2N KOH standard solution. Transmittance measurements are made with a spectrophotometer using a light of 340 mμ wave length and a cell length of 10 mm. Samples with 93-7% transmittances give pure white, polyester fibers. Cf. following abstract

IT 3766-51-6

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 3766-51-6 CAPLUS

CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)



L3 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1965:499398 CAPLUS

DN 63:99398

OREF 63:18367e-f

TI Azobenzene-containing polymeric compositions capable of being integrally colored and resistant to ultraviolet light

IN Fertig, Joseph; Goldberg, Albert I.; Skoultchi, Martin

PA National Starch and Chemical Corp.

SO 6 pp.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3190861		19650622	US 1962-205218	19620626
PRAI	US		19620626		

AB Similar to U.S. 3,190,860 (CA 63, 13529c) except that a wide variety of copolymers derived from novel azobenzene monomers are effectively stabilized against uv radiation without requiring the addition of extraneous uv absorbers to the polymer. The use of these novel monomers in higher concns. results in the preparation of copolymers which, in addition to their enhanced light stability, also have an unextractable "built in" color. The color is determined by selection of the proper azobenzene compound

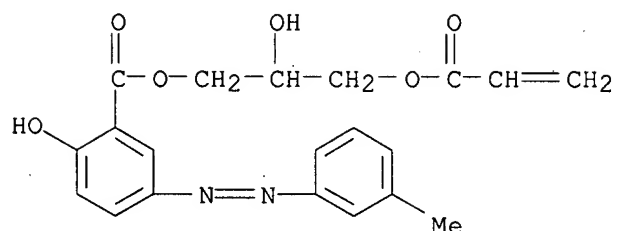
IT 3766-51-6

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 3766-51-6 CAPLUS

CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA

INDEX NAME)



L3 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1965:480362 CAPLUS

DN 63:80362

OREF 63:14761b-e

TI Ethylenically unsaturated derivatives of azobenzene

IN Skoultchi, Martin M.; Goldberg, Albert I.; Joseph Fertig

PA National Starch and Chemical Corp.

SO 5 pp.

DT Patent

LA Unavailable

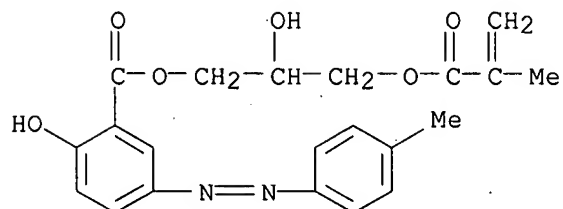
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3190874		19650622	US 1962-188861	19620419
	GB 1006884			GB	
PRAI	US		19620419		

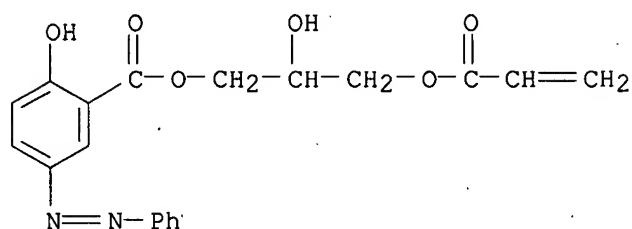
AB The title compds. were prepared by treating glycidyl acrylate or the methacrylate (I) with a carboxylated azobenzene in the presence of a catalyst. Thus, to a stirred mixture of I 156 and 50% aqueous NaOH 3.2, 5-phenylazo-2-hydroxybenzoic acid (II) 242 parts was added during 1 hr. at 70-80° the mixture stirred 7 hrs. at 70-80°, and cooled to room temperature to give 94% CH<sub>2</sub>:C(R)CO<sub>2</sub>CH<sub>2</sub>CH(OH)CH<sub>2</sub>R<sub>1</sub> (III) (R = Me, R<sub>1</sub> = 5-phenylazo-2-hydroxybenzoyloxy), tan in color but yellow-orange in organic solvents. Similarly prepared were III (R = Me) (R<sub>1</sub> and % yield given): 4-phenylazobenzoyloxy, 93; 2-phenylazobenzoyloxy, 80; 4-(4-methylphenylazo)benzoyloxy, 92; 5-(4-methylphenylazo)-2-hydroxybenzoyloxy, 94.5; 5-(3-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(2-methylphenylazo)-2-hydroxybenzoyloxy, 95; 4-(2-chlorophenylazo)benzoyloxy, 85; 4-(2-methoxyphenylazo)benzoyloxy, 86; 4-(4-phenylphenylazo)benzoyloxy, 83; 4-(2-naphthylazo)benzoyloxy, 93; and III (R = H) (R<sub>1</sub> and % yield given): 4-phenylazobenzoyloxy, 94; 2-phenylazobenzoyloxy, 83; 4-(4-methylphenylazo)benzoyloxy, 92.5; 5-(4-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(3-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(2-methylphenylazo)-2-hydroxybenzoyloxy, 95; 4-(2-chlorophenylazo)benzoyloxy, 89; 4-(2-methoxyphenylazo)benzoyloxy, 83; 4-(4-phenylphenylazo)benzoyloxy, 75; 4-(2-naphthylazo)benzoyloxy, 92. Cf. following 2 abstrs.

IT 3758-48-3P, Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-36-7P, Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-39-0P, Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-42-5P, Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-43-6P, Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-50-5P, Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-51-6P, Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-52-7P, Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate  
 RL: PREP (Preparation)  
 (preparation of)

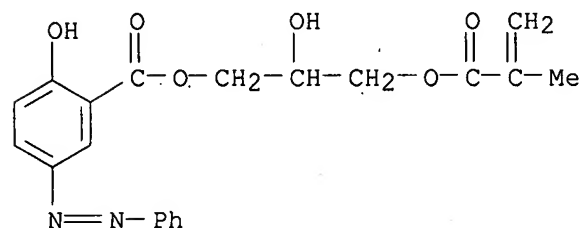
RN 3758-48-3 CAPLUS  
 CN Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate  
 (7CI, 8CI) (CA INDEX NAME)



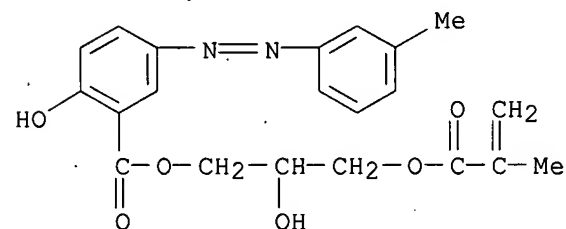
RN 3766-36-7 CAPLUS  
 CN Salicylic acid, 5-(phenylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)



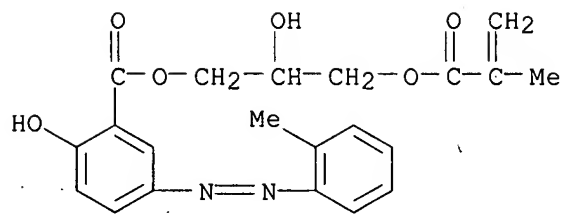
RN 3766-39-0 CAPLUS  
 CN Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate  
 (7CI, 8CI) (CA INDEX NAME)



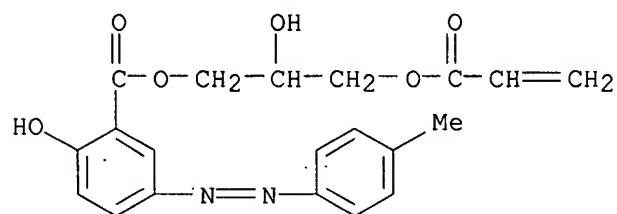
RN 3766-42-5 CAPLUS  
 CN Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate  
 (7CI, 8CI) (CA INDEX NAME)



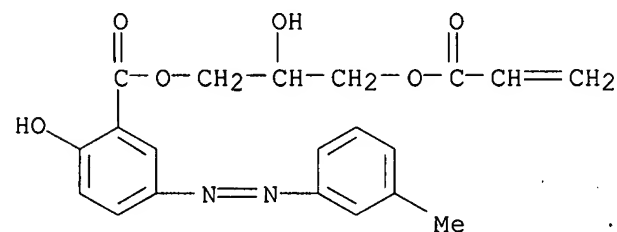
RN 3766-43-6 CAPLUS  
 CN Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate  
 (7CI, 8CI) (CA INDEX NAME)



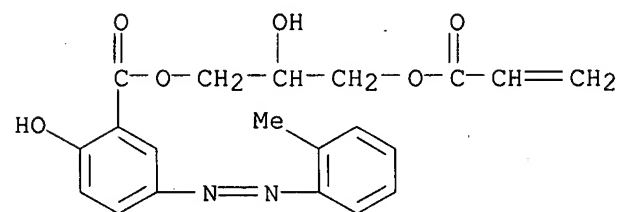
RN 3766-50-5 CAPLUS  
 CN Salicylic acid, 5-(p-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA  
 INDEX NAME)



RN 3766-51-6 CAPLUS  
 CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA  
 INDEX NAME)



RN 3766-52-7 CAPLUS  
 CN Salicylic acid, 5-(o-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA  
 INDEX NAME)



L3 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1965:2810 CAPLUS  
 DN 62:2810  
 OREF 62:464e-g  
 TI Synthesis of chloramphenicol derivatives and their preliminary  
 microbiological assay  
 AU Jaramillo, M. V. H.; v. Plessing B., Carlos

SO Farm. Nueva (Madrid) (1964), 29(329), 253-62

DT Journal

LA Spanish

GI For diagram(s), see printed CA Issue.

AB Dropwise addition of 2.2 g. salicyl chloride to a stirred cooled solution of

2.3 g. chloramphenicol in 5 ml. dioxane containing 0.5 g. NaHCO<sub>3</sub>, the mixture kept  
3 hrs. at room temperature, 100 ml. H<sub>2</sub>O containing 0.3 ml. HCl added, and the  
precipitate

collected after 2 hrs. and recrystd. from 15:3 EtOH-H<sub>2</sub>O at 60° gave  
1.522 g. white crystals. chloramphenicol (I) salicylate, m. 144-6°,

[α]<sub>D</sub><sup>18</sup>, 40.5° (absolute alc.) (ir and uv spectra given).

Sulfadiazine (3.8 g.) in 12 ml. water acidified with 4.5 ml. concentrated HCl  
was diazotized at 4° by addition of 4.3 ml. 25% NaNO<sub>2</sub> and the product

added to an ice-cold solution of 6.6 g. I in 28 ml. 9% NaOH (pH 8.0-8.5);  
after stirring 30 min., the solution was acidified to precipitate 94.7%

5-[p-(2-pyrimidinylsulfamoyl)-phenylazo]salicylate (II) of I, m.

142-3° (alc.), (α)<sub>D</sub><sup>18</sup> 71.5° (absolute alc.) (ir and uv  
spectra given). Results of pharmacol. tests were given.

IT 6868-03-7P, Salicylic acid, 5-[[p-(2-pyrimidinylsulfamoyl)phenyl]a  
zo]-, α-ester with 2,2-dichloro-N-[β-hydroxy-α-  
(hydroxymethyl)-p-nitrophenethyl]acetamide

RL: PREP (Preparation)

(preparation and bactericidal action of)

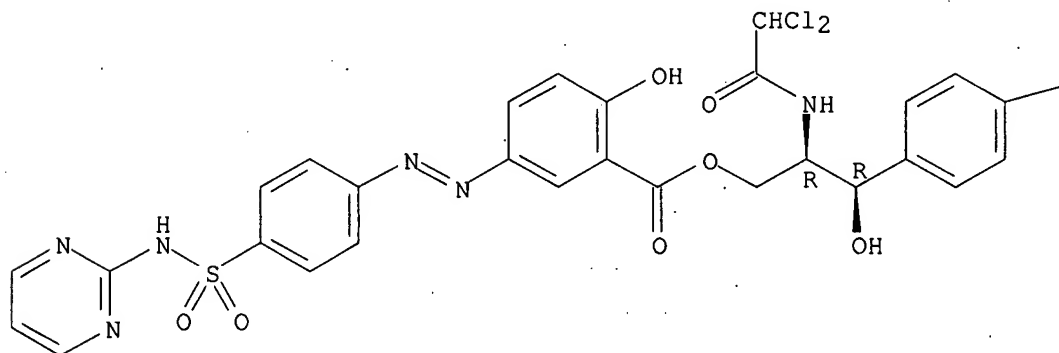
RN 6868-03-7 CAPLUS

CN Salicylic acid, 5-[[p-(2-pyrimidinylsulfamoyl)phenyl]azo]-, α-ester  
with 2,2-dichloro-N-[β-hydroxy-α-(hydroxymethyl)-p-  
nitrophenethyl]acetamide (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A



PAGE 1-B

—NO<sub>2</sub>

L3 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

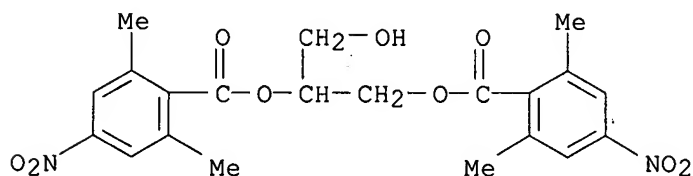
AN 1962:436109. CAPLUS

DN 57:36109

OREF 57:7162h-i

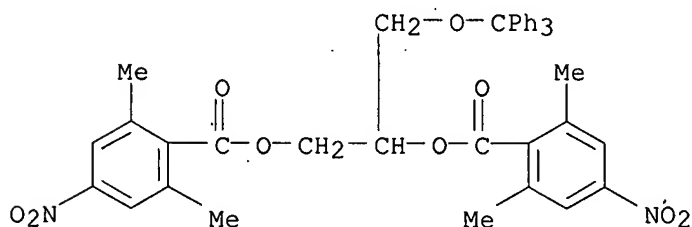
TI Chemistry of lactones. VI. Reaction of unsaturated azlactones under  
Friedel-Crafts conditions

AU Filler, Robert; Rao, Y. Shyamsunder  
 CS Illinois Inst. of Technol., Chicago  
 SO Journal of Organic Chemistry (1962), 27, 2403-6  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA Unavailable  
 AB cf. CA 55, 25906b. The behavior of unsatd. azlactones under Friedel-Crafts conditions has been studied in detail. The course of the reaction is dependent on a variety of factors, including reaction conditions, solvent, and the nature of substituents on the arylidene ring. Four different products have been isolated: saturated azlactones, w-benzamidoacetophenone, 2-benzamidoindenone, and 1-phenylisoquinoline-3-carboxylic acids.  
 IT 94862-60-9P, Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 94862-60-9 CAPLUS  
 CN Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester (7CI)  
 (CA INDEX NAME)

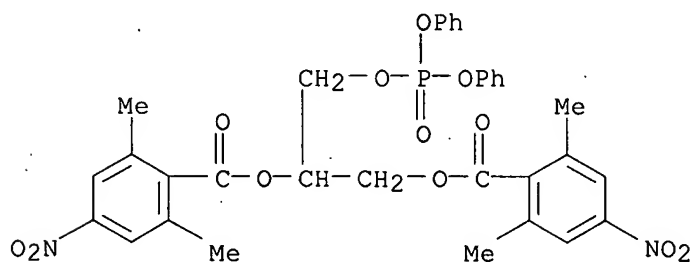


L3 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1962:436108 CAPLUS  
 DN 57:36108  
 OREF 57:7162c-h  
 TI Migration of an acyl group in glycerol derivatives. II. Transformation of diacylglycerol- $\beta$ -iodohydrins into diphenyl diacylglycerol- $\alpha$ -phosphates  
 AU Hoefnagel, M. A.; Hartman-Kohler, A. H.; Verkade, P. E.  
 CS Tech. Univ., Delft, Neth.  
 SO Recueil des Travaux Chimiques des Pays-Bas (1961), 80, 608-22  
 CODEN: RTCPA3; ISSN: 0165-0513  
 DT Journal  
 LA Unavailable  
 AB cf. CA 54, 22387h. 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>H and SOCl<sub>2</sub> (1:3) refluxed 3 hrs. gave 93% 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>COCl (I), b<sub>21</sub> 168.5-9°, m. 60.5-1.5°. To 6.73 g. HOCH<sub>2</sub>CHICH<sub>2</sub>OH (II), 30 ml. dry CHCl<sub>3</sub>, and 6 ml. dry C<sub>5</sub>H<sub>5</sub>N was added 20.3 g. C<sub>17</sub>H<sub>35</sub>COCl in 30 ml. dry CHCl<sub>3</sub> and the whole kept 4 days in the dark at 30-5° to give 28.8 g. C<sub>17</sub>H<sub>35</sub>CO<sub>2</sub>CH<sub>2</sub>CHICH<sub>2</sub>O<sub>2</sub>CC<sub>17</sub>H<sub>35</sub> (IIa), m. 57-8° (petr. etherabs. MeOH). To 8.08 g. HOCH<sub>2</sub>CH(OH)CH<sub>2</sub> (III), 40 ml. dry C<sub>6</sub>H<sub>6</sub>, and 12 ml. pure Et<sub>3</sub>N was added 13.92 g. p-MeOC<sub>6</sub>H<sub>4</sub>COCl (IIIa), and the whole kept 6 days in the dark at room temperature gave 16.72 g. p-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH (O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p)CH<sub>2</sub> (IV), m. 94-5° (C<sub>6</sub>H<sub>6</sub>-petr. ether); II similarly gave 98% p-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CHICH<sub>2</sub>O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p (V), m. 69-70° (EtOAc-MeOH); II and I gave 93% 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>CHICH<sub>2</sub>O<sub>2</sub>CC<sub>6</sub>(O<sub>2</sub>N)Me<sub>2</sub>-4,6,2 (VI), m. 154-5° (C<sub>6</sub>H<sub>6</sub>-MeOH); I and III gave a poor yield of 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>CH<sub>2</sub>CH[O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(O<sub>2</sub>N)Me<sub>2</sub> 4,6,2]CH<sub>2</sub>I (VII), m. 174.5-5.5° (EtOAcMeOH). IIa (2.49 g.), 60 ml. C<sub>6</sub>H<sub>6</sub>, and 1.57 g. (PhO)<sub>2</sub>-PO(OAg) (VIII) refluxed 6 hrs. gave 3.22 g.  $\alpha$ -phosphate derivative, m. 58-9° (petr. ether); in similar fashion, IV and VIII gave 94% of  $\alpha$ -phosphate (IX), m. 64-6.5° (Et<sub>2</sub>Opetr. ether); V and VIII also gave IX; both VI and VII with VIII gave the

$\alpha$ -phosphate (X), m. 112-13° (MeOH). To Ph<sub>3</sub>COCH<sub>2</sub>CH(OH)CH<sub>2</sub>OH (XI) in 15 ml. dry C<sub>5</sub>H<sub>5</sub>N was added 6.0 g. IIIa and the whole kept several days at room temperature gave 92% Ph<sub>3</sub>COCH<sub>2</sub>CH(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p)CH<sub>2</sub>O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p (XII), m. 134.5-5° (EtOAc-petr. ether); alternately, 2.55 g. p-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p)CH<sub>2</sub>OH (XIII), 2.42 g. Ph<sub>3</sub>CBr (XIV) and 35 ml. dry C<sub>5</sub>H<sub>5</sub>N kept 8 hrs. at 100° gave 3.49 g. XII. XI (1.67 g.), 2.3 g. I, and 30 ml. pure Et<sub>3</sub>N kept 12 days at room temperature gave 1.50 g. Ph<sub>3</sub>COCH<sub>2</sub>CH[O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(O<sub>2</sub>N)Me<sub>2</sub>-4,6,2]CH<sub>2</sub>O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(O<sub>2</sub>N)Me<sub>2</sub>-4,6,2 (XV), m. 172-3°; alternately, XIV and 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>CH[O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(NO<sub>2</sub>)Me<sub>2</sub>-4,6,2]CH<sub>2</sub>OH, as above, also gave XV. XII (12.04 g.), 200 ml. absolute EtOH, and Pd-C (from 1 g. PdCl<sub>2</sub>) shaken 5 hrs. at 65-75° with H<sub>2</sub>, the whole filtered, the EtOH distilled and the residue dissolved in 180 ml. petr. ether gave 6.73 g. p-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OMe-p)CH<sub>2</sub>OH, m. 62.5-3.5°. At 0°, to 2.05 g. XV in 3 ml. C<sub>6</sub>H<sub>6</sub> and 5 ml. glacial AcOH was added 6 ml. HBr saturated AcOH, the whole kept 5 min. at 0° the XIV filtered, the filtrate in 125 ml. Et<sub>2</sub>O washed with H<sub>2</sub>O, 5% KHC<sub>3</sub>O<sub>3</sub>, dried, and concentrated gave 1.13 g. 2,6,4-Me<sub>2</sub>(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>CH<sub>2</sub>CH[O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(NO<sub>2</sub>)Me<sub>2</sub>-4,6,2]CH<sub>2</sub>OH, m. 138-9° (C<sub>6</sub>H<sub>6</sub>-MeOH).  
 IT 96871-82-8P, Benzoic acid, 2,6-dimethyl-4-nitro-, [(trityloxy)methyl]ethylene ester 97658-12-3P, Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester, di-Ph phosphate  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 96871-82-8 CAPLUS  
 CN Benzoic acid, 2,6-dimethyl-4-nitro-, [(trityloxy)methyl]ethylene ester (7CI) (CA INDEX NAME)



RN 97658-12-3 CAPLUS  
 CN Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester, diphenyl phosphate (7CI) (CA INDEX NAME)



L3 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1954:25061 CAPLUS  
 DN 48:25061  
 OREF 48:4548b-d  
 TI Less known properties of nitro compounds  
 AU Urbanski, Tadeusz  
 CS Inst. Technol., Warsaw  
 SO Roczniki Chemii (1951), 25, 257-84;English summary, 284-6

CODEN: ROCHAC; ISSN: 0035-7677

DT Journal

LA Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 46, 7993c. A review of chemical properties of nitro compds. is presented. Unpublished so far, the preparation of a number of pyrimidine compds.

of the type (I) from MeNO<sub>2</sub> is mentioned; also a tetrahydrooxazine compound (II) was obtained from PhCH<sub>2</sub>NO<sub>2</sub>.

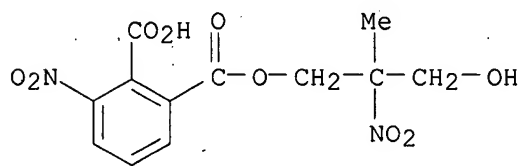
IT 856806-60-5P, Phthalic acid, 3-nitro-, ester with 2-methyl-2-nitro-1,3-propanediol

RL: PREP (Preparation)

(preparation of)

RN 856806-60-5 CAPLUS

CN Phthalic acid, 3-nitro-, ester with 2-methyl-2-nitro-1,3-propanediol (5CI)  
(CA INDEX NAME)





JC 6/20/07

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NEWS 13 MAY 08 CA/CAPplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
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AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.  
  
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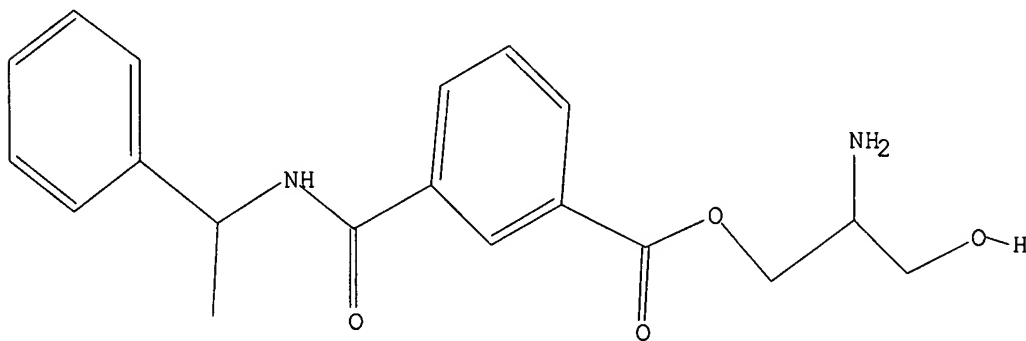
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0 ANSWERS

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BATCH \*\*COMPLETE\*\*

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PROJECTED ANSWERS: 0 TO 0

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100.0% PROCESSED 116 ITERATIONS

5 ANSWERS

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L3 5 SEA SSS FUL L1

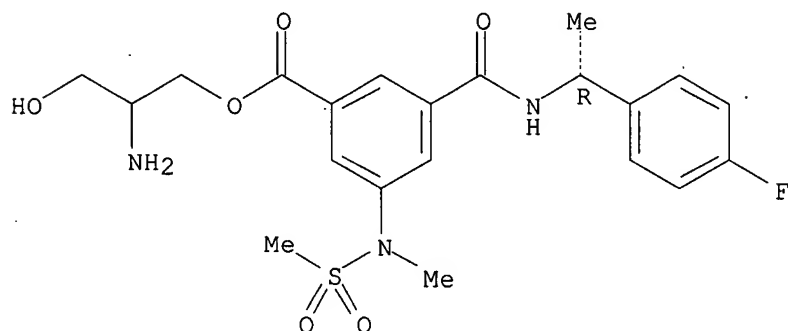
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L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI)

MF C21 H26 F N3 O6 S

Absolute stereochemistry.



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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26

FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/infopolicy.html>

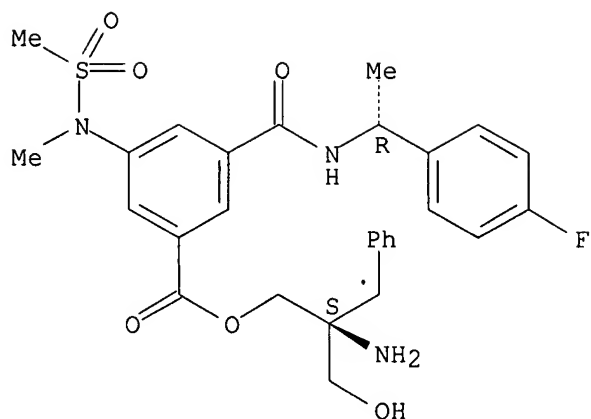
=> s 13

L4 2 L3

=> d 14 1-2 bib abs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2006:1191598 CAPLUS  
DN 146:116781  
TI Discovery of Oxadiazoyl Tertiary Carbinamine Inhibitors of  
 $\beta$ -Secretase (BACE-1)  
AU Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi,  
Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth;  
Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis;  
Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian;  
Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel;  
Vacca, Joseph P.  
CS Departments of Medicinal Chemistry, Structural Biology, Molecular Systems  
and Alzheimer's Research, Merck Research Laboratories, West Point, PA,  
19486, USA  
SO Journal of Medicinal Chemistry (2006), 49(25), 7270-7273  
CODEN: JMCMAR; ISSN: 0022-2623  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 146:116781  
AB We describe the discovery and optimization of tertiary carbinamine derived  
inhibitors of the enzyme  $\beta$ -secretase (BACE-1). These novel  
non-transition-state-derived ligands incorporate a single primary amine to  
interact with the catalytic aspartates of the target enzyme. Optimization  
of this series provided inhibitors with intrinsic and functional potency  
comparable to evolved transition state isostere derived inhibitors of  
BACE-1.  
IT 918344-77-1 918344-77-1D, complexes with  
 $\beta$ -secretase  
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL  
(Biological study)  
(discovery of oxadiazoyl tertiary carbinamine inhibitors of  
 $\beta$ -secretase)  
RN 918344-77-1 CAPLUS  
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-  
[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-  
phenylpropyl ester (CA INDEX NAME)

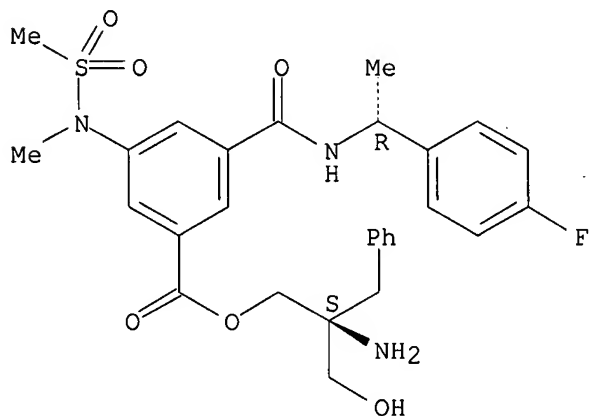
Absolute stereochemistry.



RN 918344-77-1 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:55021 CAPLUS

DN 142:134323

TI Preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease

IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DT Patent

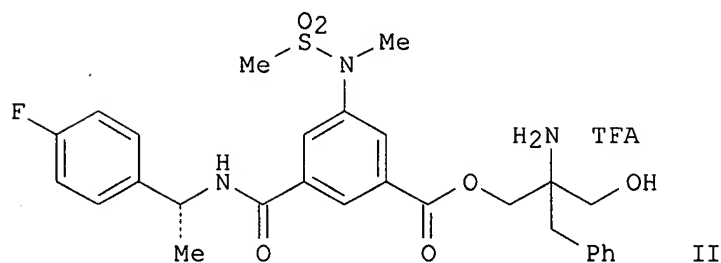
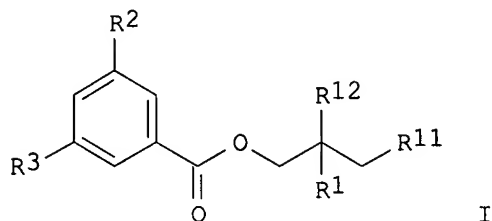
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,				

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
 SN, TD, TG

AU 2004255191 A1 20050120 AU 2004-255191 20040625  
 CA 2530006 A1 20050120 CA 2004-2530006 20040625  
 EP 1643986 A2 20060412 EP 2004-756168 20040625  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK  
 CN 1909897 A 20070207 CN 2004-80018651 20040625  
 US 2006149092 A1 20060706 US 2005-562470 20051222  
 PRAI US 2003-484150P P 20030701  
 WO 2004-US20525 W 20040625  
 OS MARPAT 142:134323  
 GI



AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidiny, piperidiny; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

IT 827039-53-2P 827039-54-3P

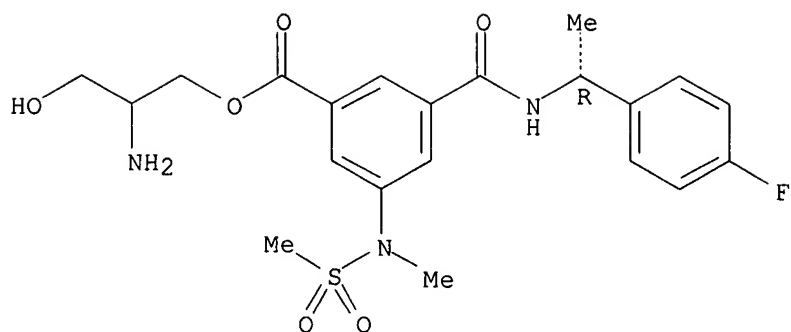
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-53-2 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI) (CA INDEX NAME)

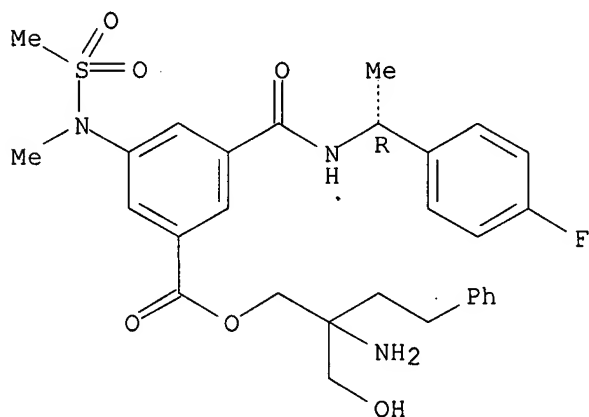
Absolute stereochemistry.



RN 827039-54-3 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-4-phenylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 827039-74-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-74-7 CAPLUS

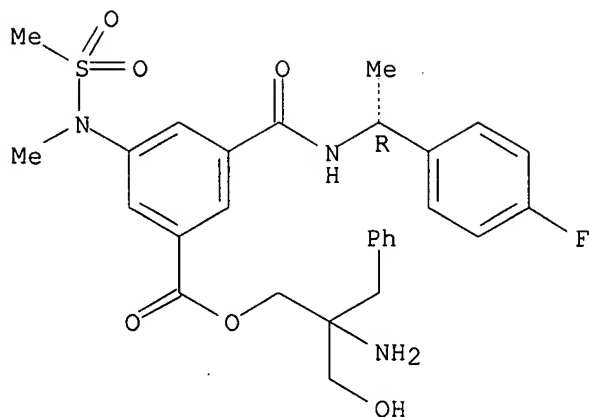
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 827039-73-6

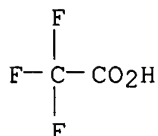
CMF C28 H32 F N3 O6 S

Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2



=> file registry  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
11.48	184.45

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.56	-1.56

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 09:57:29 ON 20 JUN 2007  
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DICTIONARY FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:



<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\jcho2\My Documents\10562470-a.str

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 15 sss sam

SAMPLE SEARCH INITIATED 09:58:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1 TO 80

PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 09:58:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

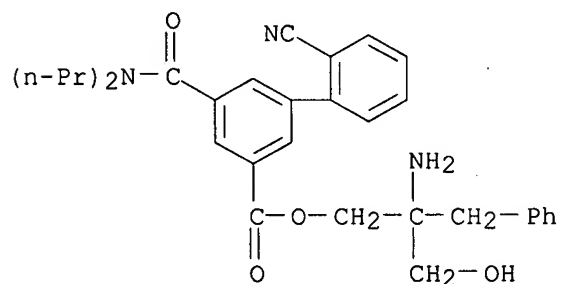
L7 2 SEA SSS FUL L5

=> d scan

L7 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-,  
2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI)

MF C31 H35 N3 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

173.00

357.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-1.56

FILE 'CAPLUS' ENTERED AT 09:59:09 ON 20 JUN 2007

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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26

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=> s 17

L8 1 L7

=> d 18 bib abs hitstr

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:55021 CAPLUS

DN 142:134323

TI Preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease

IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DT Patent

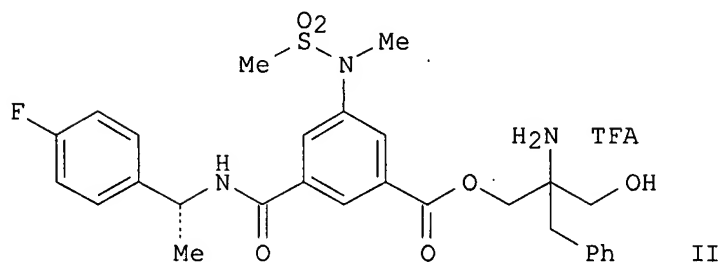
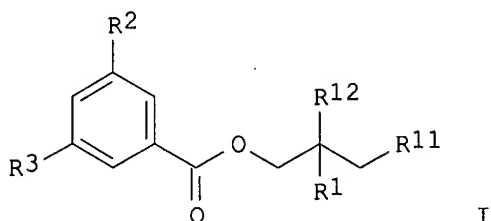
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,				

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
SN, TD, TG

AU 2004255191	A1	20050120	AU 2004-255191	20040625
CA 2530006	A1	20050120	CA 2004-2530006	20040625
EP 1643986	A2	20060412	EP 2004-756168	20040625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1909897	A	20070207	CN 2004-80018651	20040625
US 2006149092	A1	20060706	US 2005-562470	20051222
PRAI US 2003-484150P	P	20030701		
WO 2004-US20525	W	20040625		
OS MARPAT 142:134323				
GI				



AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidiny, piperidiny; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

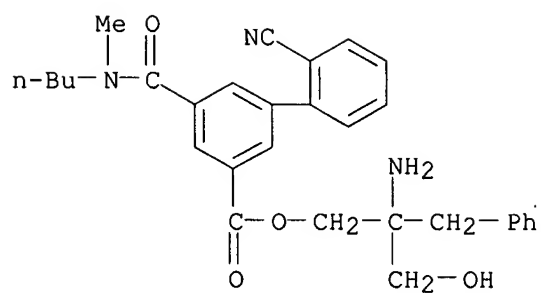
IT 827039-57-6P 827039-62-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease)

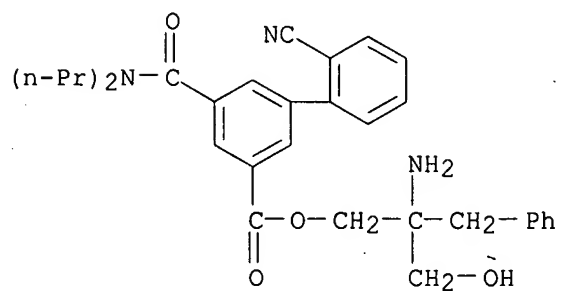
RN 827039-57-6 CAPLUS

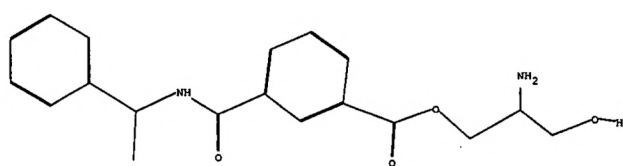
CN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)

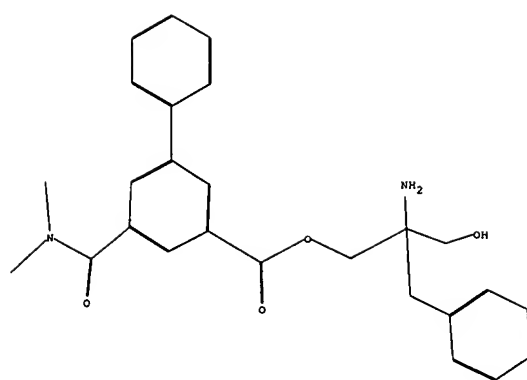


RN 827039-62-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)







Connecting via Winsock to STN

JC 6/20/07  
STN SSS search.

Welcome to STN International! Enter x:x

LOGINID:SSPTAJYC1621

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'REGISTRY' AT 10:32:39 ON 20 JUN 2007  
FILE 'REGISTRY' ENTERED AT 10:32:39 ON 20 JUN 2007  
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COST IN U.S. DOLLARS

	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.90	1.11

=> file registry

	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.90	1.11

FILE 'REGISTRY' ENTERED AT 10:32:52 ON 20 JUN 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1  
DICTIONARY FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1

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predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

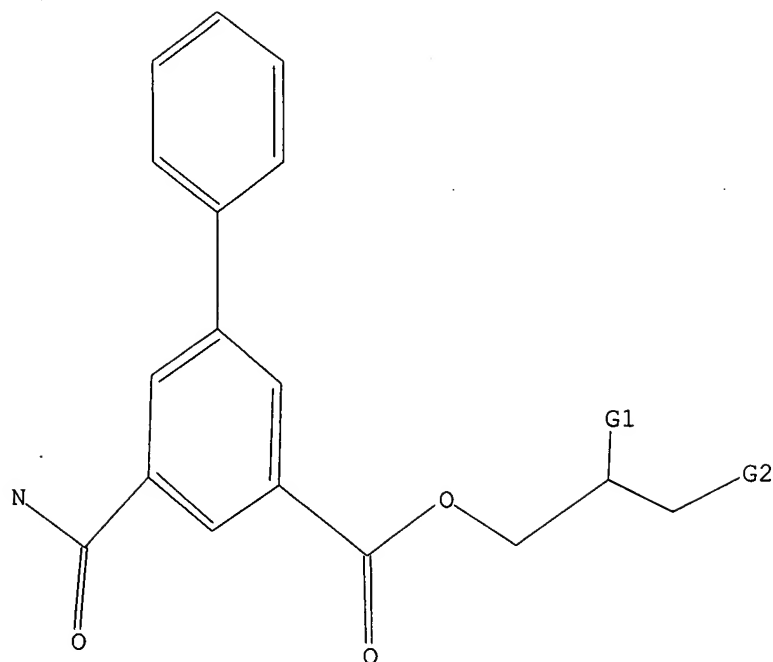
Uploading C:\Documents and Settings\jcho2\My Documents\10562470-e.str

L2 STRUCTURE UPLOADED

=> d ll

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

SEARCH FAILED DUE TO A STRUCTURE QUERY ERROR

The structure query could not be searched. Please review and revise your structure query, especially checking the variable definitions and attachments. In rare instances the failure may be due to a system problem. Please contact your local STN Help Desk if you need assistance.

=>

Uploading C:\Documents and Settings\jcho2\My Documents\10562470-f.str

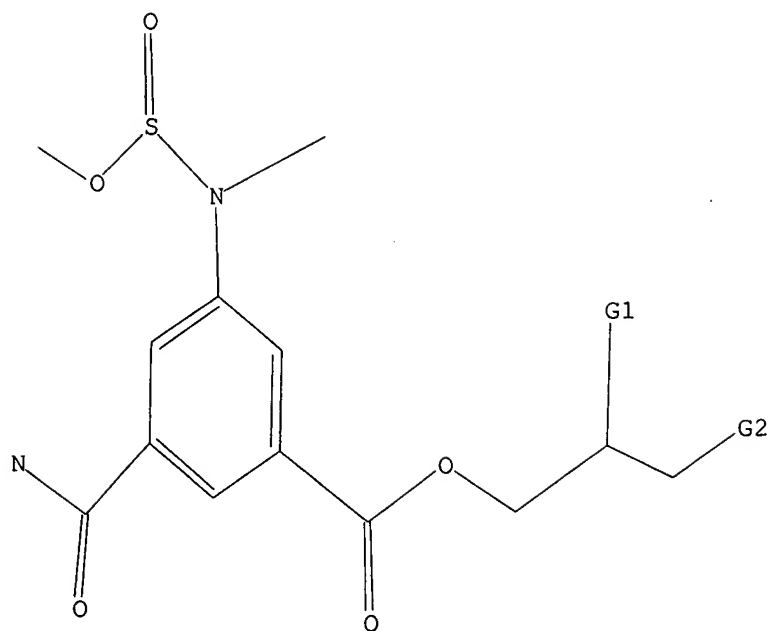
L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR





G1 O,N  
G2 Ph,O

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

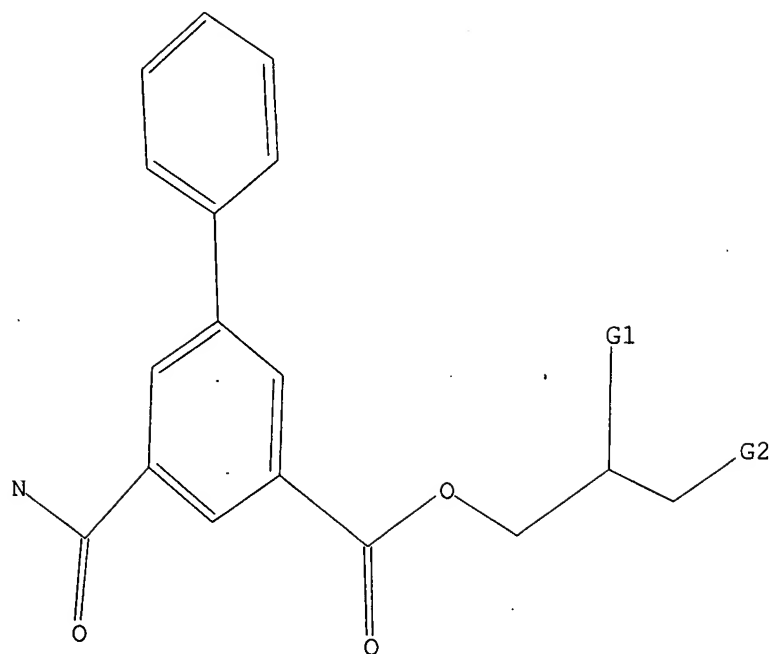
100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L3

=>  
Uploading C:\Documents and Settings\jcho2\My Documents\10562470-g.str

L5 STRUCTURE UPLOADED

=> d l5  
L5 HAS NO ANSWERS  
L5 STR



G1 O,N  
G2 Ph,O

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 23 TO ITERATE

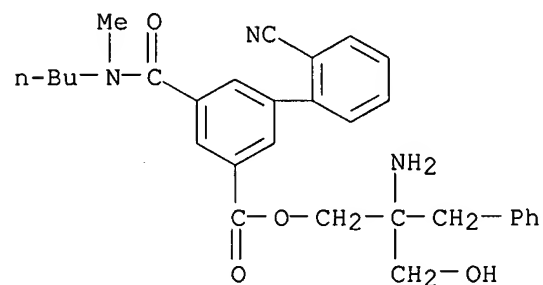
100.0% PROCESSED 23 ITERATIONS  
SEARCH TIME: 00.00.01

2 ANSWERS

L6 2 SEA SSS FUL L5

=> d scan

L6 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-  
, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI)  
MF C30 H33 N3 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

346.00

347.11

FILE 'CAPLUS' ENTERED AT 10:36:14 ON 20 JUN 2007

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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26

FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

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=> s l2

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 10:36:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED

2 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 1 TO 80

L7 1 SEA SSS SAM L2

L8 1 L7

=> s l6

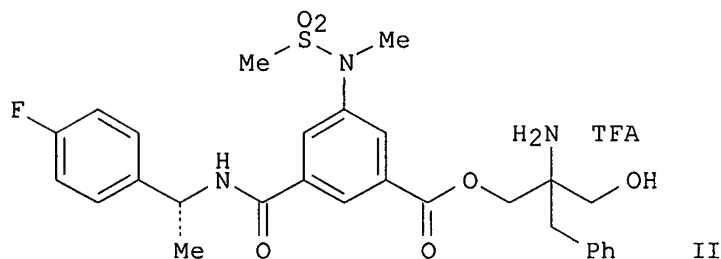
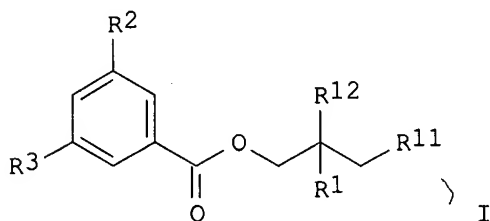
L9 1 L6

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L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:55021 CAPLUS  
 DN 142:134323  
 TI Preparation of phenylcarboxylate esters as  $\beta$ -secretase inhibitors for the treatment of Alzheimer's disease  
 IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004255191	A1	20050120	AU 2004-255191	20040625
	CA 2530006	A1	20050120	CA 2004-2530006	20040625
	EP 1643986	A2	20060412	EP 2004-756168	20040625
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1909897	A	20070207	CN 2004-80018651	20040625
	US 2006149092	A1	20060706	US 2005-562470	20051222
PRAI	US 2003-484150P	P	20030701		
	WO 2004-US20525	W	20040625		
OS	MARPAT 142:134323				
GI					



AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl,

alkenyl, alkynyl, Ph, PhCH<sub>2</sub>; R<sub>7</sub> = H, alkyl, alkenyl, alkynyl; R<sub>3</sub> = (substituted) PhCHR<sub>5</sub>NHCO, R<sub>9</sub>R<sub>10</sub>NHCO, etc.; R<sub>9</sub>R<sub>10</sub> = atoms to form (substituted) pyrrolidinyl, piperidinyl; R<sub>11</sub> = OH, alkoxy, phenylalkoxy, PhO, Ph; R<sub>12</sub> = NR<sub>9</sub>R<sub>10</sub>, OH], were prepared as β-secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

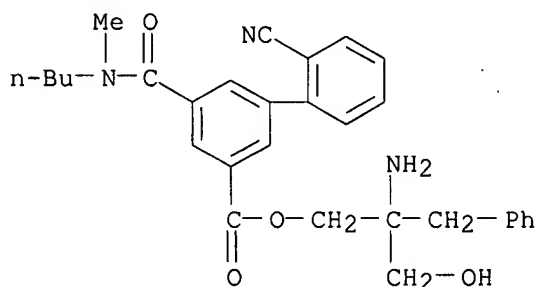
IT 827039-57-6P 827039-62-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

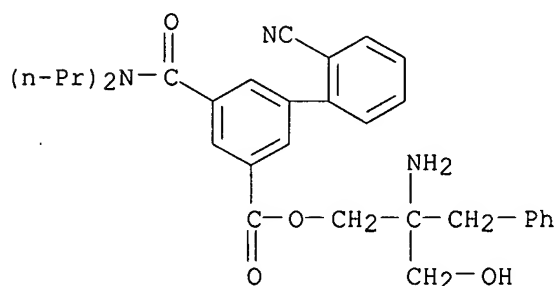
RN 827039-57-6 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)



RN 827039-62-3 CAPLUS

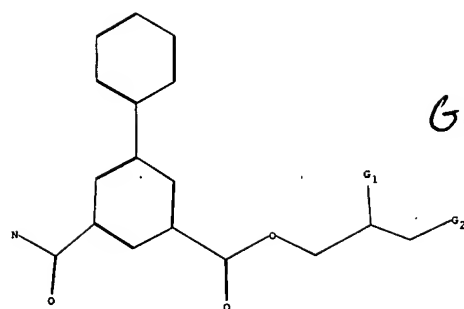
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)



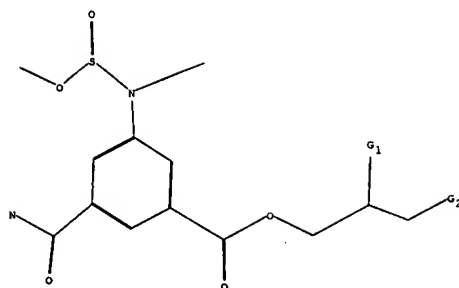
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L10

0 L4



$G_1 = N, O$   
 $G_2 = O$  Phenyl



$G_1 = N, O$

$G_2 = O, \text{Phenyl}$